FACULTY OF SCIENCE,
HUMANITIES AND
EDUCATION TUL

Dissertation

THE CORE PROBLEM --- ANALYSIS, PROPERTIES, AND BEHAVIOUR

Study programme:	P1103 – Applied mathematics
Study branch:	1103V035 – Mathematical models and their applications
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Liberec 2023

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THE CORE PROBLEM --- ANALYSIS, PROPERTIES, AND BEHAVIOUR

ABSTRACT

A wide range of problems arising in real-world applications needs to be solved as linear approximation problems, since they might contain some errors in data. This thesis focuses on solving such problems with the method of the total least squares and the reduction to the so-called core problem within, which is briefly recapitulated in Part I. Although the core problem concept brought important results on solvability of the vector right-hand side problem, it is not completely true for the problem with matrix right-hand side as the core problem within may not have a TLS solution. Therefore, this thesis aims to examine the '*internal structure*' of the matrix right-hand side core problems as well as to '*look around*' this problem in order to find possible generalizations.

In Part II we build general algebraic framework, which enables to interpret the core problem reduction as the orthogonal projection from the set of general approximation problems onto the set of core problems and partially open the question of the core problem (de)composition and (ir)reducibility.

Part III extends the core problem theory with three possible generalizations, namely we present the core problem reductions within the linear approximation problem with tensor right-hand side, the bilinear problem with matrix right-hand side and the multilinear problem with tensor right-hand side. The text of this thesis is complemented by copies of the relevant published articles of the applicant.

Keywords: linear approximation problem; total least squares; core problem; core problem reduction; orthogonal transformation; matrix right-hand side; problem (de)composition; irreducible problem; tensor; tensor right-hand side; bilinear problem; multilinear problem

ACKNOWLEDGEMENTS

I could not have undertaken this journey without the careful supervision of Martin Plešinger, who invested a lot of energy and time to our common projects as well as to consultations about this thesis. Special thanks to our co-author Iveta Hnětynková for her long-term cooperation and valuable advice.

Thanks should also go to my colleagues from Department of Mathematics, Technical University of Liberec, for constituting the pleasant working environment and being the source of inspiration and help.

I am also grateful to my family and my boyfriend Marek as their belief in me has kept my motivation to accomplish the studies even in tougher whiles. Lastly, I would like to thank my friends for the pleasant distraction from the academic world and their emotional support.

CONTENTS

NOTATION & ABBREVIATIONS

$\mathbb{N}$, $\mathbb{N}_0$	semi-rings of positive and non-negative integers
$\mathbb{R}$	field of real numbers
$\mathbb{C}$	field of complex numbers
$\mathbb{F}$	field of real or complex numbers; either $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$
$\mathbb{R}^n$	vector space of real vectors of length n
$\mathbb{R}^{m \times n}$	vector space of real m-by-n matrices
$\mathbb{R}^{m_1 \times \cdots \times m_k}$	vector space of real k-way tensors
$\mathbb{O}$, $\mathbb{O}_m$	group of orthogonal matrices, ditto of dimension m
$\mathbb{U}$, $\mathbb{U}_m$	group of unitary matrices, ditto of dimension m
$\mathscr{M}$, $\mathscr{M}(\mathbb{R})$	the set of all real matrices
$\mathbb{CP}$	the set of all core problems
$\mathbb{GP}$	the set of all general (linear approximation) problems
v^T	transposition of the vector v (treated as n-by-1 matrix)
M^T	transposition of the matrix M
M^H	Hermitian transposition of the matrix M; $M^\mathsf{H} = \overline{M}^\mathsf{T}$
M^{-1}	inverse of the matrix M
$M^\dagger$	Moore–Penrose pseudoinverse of the matrix M
$\mathcal{R}(M)$	range of the matrix M
$\mathcal{N}(M)$	null-space of the matrix M
dim$(\mathscr{V})$	dimension of linear vector space $\mathscr{V}$
$\sim$	similarity relation
$\perp$	orthogonality relation
$\lVert v \rVert$	2-norm of the vector v
$\lVert M \rVert_\mathsf{F}$	Frobenius norm of the matrix M
det(M)	determinant of the square matrix M
rank(M)	rank of the matrix M
$\sigma_j(M)$	jth largest singular value of the matrix M
I, I_m	identity matrix, ditto of order m
$0_{m,n}$	m-by-n zero matrix
$0_{m_1,\ldots,m_k}$	zero tensor of order k
$\heartsuit$	number (entry) that may be zero as well as nonzero
$\clubsuit$	number (entry) that is nonzero

$M \otimes N$	Kronecker product of matrices M and N
$M \oplus N$	2-by-2 (block) diagonal matrix with M and N on diagonal
diag(M, N)	2-by-2 (block) diagonal matrix with M and N on diagonal
diag$_k(\mathcal{T}, \mathcal{N})$	analogy of diag for tensors of order k
$\mathcal{T}^{\{\ell\}}$	ℓ-mode matricization of the tensor $\mathcal{T}$
$M \times_\ell \mathcal{T}$	ℓ-mode matrix-tensor product; $(M \times_\ell \mathcal{T})^{\{\ell\}} = M\mathcal{T}^{\{\ell\}}$
$(M_1, \ldots, M_k \vert \mathcal{T})$	linear transformation of $\mathcal{T}$; $(M_1, \ldots, M_k \vert \mathcal{T}) = M_1 \times_1 \ldots M_k \times_k \mathcal{T}$

SVD	singular value decomposition
HOSVD	high-order SVD (Tucker decomposition)
TC	Tucker core from the Tucker decomposition
TLS	total least squares (minimization, solution, etc...)
NGN	non-generic (TLS approach, solution, etc...)
CP	core problem
CPℓ	the ℓth core problem property
CPR	core problem reduction
CPC	core problem complement
GP	general (linear approximation) problem
TA	tuple alignment (set of conditions on dimensions)
TM	tuple matricization (mapping from $\mathscr{M}^{\zeta}$ to $\mathscr{M}$)
TT	tuple transformation (group of allowed transformations)

INTRODUCTION

Linear approximation problems, which can be seen as problems contaminated by some errors in data, have been intensively studied during last decades as they very often yield from some real-world applications. Since such problems cannot be solved without some corrections, some appropriate method (very often a kind of the least squares methods) has to be used. We are in particular interested in solving such problems in the sense of the total least squares (TLS), but other orthogonally invariant optimizations are also relevant. The TLS method allows to correct the right-hand side (observed data) of the problem, as well as the system matrix (the mapping) in order to achieve the solution of the modified problem and consequently the approximate solution of the original problem. The simplest variants of such problems are linear approximation problems with single (or vector) right-hand side and with multiple (or matrix) right-hand side, respectively. For the above mentioned approximation problems there exist a lot of theory including the algorithms and solvability analysis, e.g., in [2] some aspects in solvability analysis for TLS problems for the vector right-hand side case can be found, or in [30] both vector and matrix right-hand side cases are studied. However, there were still many things unclear — the main difficulty of the TLS approach is the fact that some problems may not have a solution; see [5]. Note that although the TLS theory was studied since 1980s, it is still in the interest of many research directions. For example TLS minimization with arbitrary unitarily invariant norms is studied in [32]; conditioning of the TLS is studied in [13], [19], or [35]; different computational methods are studied, see [31] for quantum algorithm, or [33] and [36] for randomized algorithms. Here we are interested in the so-called core problem within the TLS minimization.

The core problem concept introduced by Paige and Strakoš (see [22]) brought important insight to the solvability of problems with vector right-hand side case. The core problem is defined as a minimal dimensioned subproblem of the original problem containing all the necessary and sufficient information for finding the solution of the whole problem, which moreover can be reached by orthogonal transformations. The key property of the core problem within problems with vector right-hand side is that it always has the unique TLS solution (see [22]). Representation of this TLS solution (of the core problem) in the context of the original problem then depends on its properties. In this way the core problem allows to explain when the original problem has TLS solution and when does not.

Successively, the core problem concept was generalized for the problems with matrix right-hand sides (see [6] and [7]) including the analysis of solvability (see [4]) of core problems with multiple right-hand sides in the TLS sense. It was shown that, contrary to the single right-hand side case, a core problem with multiple right-hand sides may not have a TLS solution. The straightforward question: *'Why is it so?'* led to the natural consideration of directions of further research. The first one is to look inside the core problem and to try to find some internal structure, the second one is to look at the core problems from the wider context and try to find possible ways of further generalization. Both of these ways are covered in this thesis.

This thesis is organized in three main parts, after this Introduction Part I summarizes basics about linear approximation problems and the well-known facts and results about the total least squares (TLS) methods (in particular Chapter 1 discusses the so-called vector and matrix right-hand side problems, Chapter 2 then formulates an interesting open question related to the matrix right-hand side core problems while motivating two ways of the further analysis). Parts II and III then represent these two ways that we call: the inner and the outer view — looking inside and around the core problems, respectively. The thesis is enclosed by Conclusion and a brief curriculum vitæ of the applicant.

Part II consists of three chapters: Chapter 3 analyzes several algebraic structures in the set of all matrices related to direct summation and orthogonal transformations in order to introduce useful concepts, notation, and terminology. Chapter 4 then generalizes these concepts to tuples of matrices and so-called aligned tuples — tuples that can be matricized in a nontrivial way and also orthogonally transformed in this matricized form. Chapter 5 finally applies these concept to special cases of aligned tuples — data matrices $[B, A]$ of linear approximation problems $AX \approx B$. This enables to better understand (de)composing and (ir)reducibility of core problems.

Part III consists of four chapters. Chapter 6 briefly recapitulates the relationships (in terms of generalizations and specializations) among individual linear approximation problems. The remaining three chapters discuss (the linear approximation problem, the TLS minimization, the core problem reduction and its properties for) the individual formulations: Chapter 7 for the tensor right-hand side case; Chapter 8 for the bilinear case with matrix right-hand side; and Chapter 9 for the k-linear case with tensor right-hand side.

Each of the individual parts ends with the copy of related published works of the applicant: Part I is enclosed by a very brief two-pages contribution which represents rather minor result (but anyway related to the topic). The main results are presented in four papers enclosing Parts II (one paper) and III (three papers).

PART I

BASIC LINEAR APPROXIMATION PROBLEMS AND THE TOTAL LEAST SQUARES METHOD

1 INTRODUCTION TO LINEAR APPROXIMATION PROBLEMS

Linear approximation problems appear in many real-world applications, see for example [28], [29]. They typically have the form of a '*system of linear equations*' but without the solution in the classical meaning, i.e., the equality cannot be reached as the right-hand side is not in the range of the system matrix. Thus, it does not represent a linear system in fact, but the problem has to be treated via some kind of minimization process — usually some form of least squares technique; see [18], [1], [3, Chaps. 5 and 6]. Here we focus on the so-called *total least squares* (TLS) minimization; see for example [2], [30], [3, Sec. 6.3]. The so-called *core problem reduction* (CPR) is a well-established concept for solving the linear approximation problems by using the TLS method in the simplest case; see [21], [22].

In this chapter we start with a brief recapitulation of the theory. We introduce the TLS formulation for the simplest (namely the vector right-hand side) linear approximation problem and describe the reduction of the original problem to the core problem within. We remind how the core problem concept clarified the solvability of the TLS problem in the vector right-hand side case. We also briefly recapitulate and point out difficulties of its most straightforward generalization — the matrix-right hand side case.

1.1 PROBLEM WITH SINGLE (VECTOR) RIGHT-HAND SIDE

The simplest case of linear approximation problems is a problem with a vector on the right-hand side, i.e.,

$$Ax \approx b, \qquad A \in \mathbb{R}^{m\times n}, \quad b \in \mathbb{R}^m \quad \text{such that} \quad b \notin \mathcal{R}(A). \tag{1.1}$$

The last condition simply says, that there is no vector x for which $Ax = b$. This may happen, e.g., due to contamination of real application data $[b, A]$ by some errors. Instead, we seek for some '*completely different*' x, that allows to equalize the left- and right-hand sides at least approximately. The way of the approximation, however, needs to be specified; for example, one can minimize the 2-norm of residuum $b - Ax$, yielding the ordinary least squares solution.

1.1.1 Total least squares and its orthogonal invariance

By solving the linear approximation problem (1.1) in the sense the total least squares (TLS) we mean solving the following minimization problem

$$\min_{E,\,g} \left\| [\, g \,|\, E \,] \right\|_{\mathsf{F}} \qquad \text{subject to} \qquad (b+g) \in \mathcal{R}(A+E). \tag{1.2}$$

Then by the TLS solution we mean any vector x_{TLS} such that

$$(A+E)x_{\mathsf{TLS}} = (b+g). \tag{1.3}$$

Since the Frobenius norm is orthogonally invariant, Paige and Strakoš (see [21], [22]) pointed out that any orthogonal transformation of the problem does not affect the solution in the following sense.

First, let us denote by

$$\mathbb{O}_m = \{ P \in \mathbb{R}^{m\times m} \ : \ P^{-1} = P^{\mathsf{T}} \} \tag{1.4}$$

the set of all orthogonal matrices of order m. For any two orthogonal matrices $P \in \mathbb{O}_m$ and $Q \in \mathbb{O}_n$, the original problem $Ax \approx b$ can be transformed into a tilded one

$$\widetilde{A}\widetilde{x} \;=\; (P^{\mathsf{T}}AQ)(Q^{\mathsf{T}}x) \approx (P^{\mathsf{T}}b) \;=\; \widetilde{b},$$

where $\widetilde{A} \equiv P^{\mathsf{T}}AQ$, $\widetilde{x} \equiv Q^{\mathsf{T}}x$ and $\widetilde{b} \equiv P^{\mathsf{T}}b$; equivalently

$$[\,\widetilde{b}\,|\,\widetilde{A}\,]\begin{bmatrix}-1\\ \widetilde{x}\end{bmatrix} = \left(P^{\mathsf{T}}\ [\,b\,|\,A\,]\left[\begin{array}{c|c}1&0\\\hline 0&Q\end{array}\right]\right)\left(\left[\begin{array}{c|c}1&0\\\hline 0&Q^{\mathsf{T}}\end{array}\right]\begin{bmatrix}-1\\ x\end{bmatrix}\right) \approx 0.$$

Let for the given A and b exist $E = E(A,b)$, $g = g(A,b)$ satisfying (1.2), and therefore also $x_{\mathsf{TLS}} = \mathsf{TLS}(A,b)$ satisfying (1.3). Then, by the multiplication of the equality (1.3) by P and Q

$$\Big(P^{\mathsf{T}}(A+E)Q\Big)\,\Big(Q^{\mathsf{T}}x_{\mathsf{TLS}}\Big) = \Big(P^{\mathsf{T}}(b+g)\Big),$$

we immediately get $\widetilde{E} = P^{\mathsf{T}}EQ = E(\widetilde{A},\widetilde{b})$, $\widetilde{g} = P^{\mathsf{T}}g = g(\widetilde{A},\widetilde{b})$, and $\widetilde{x}_{\mathsf{TLS}} = Q^{\mathsf{T}}x_{\mathsf{TLS}} = \mathsf{TLS}(\widetilde{A},\widetilde{b})$ for the tilded problem. It follows directly from the fact that

$$\left\| [\,\widetilde{g}\,|\,\widetilde{E}\,] \right\|_{\mathsf{F}} = \left\| P^{\mathsf{T}}\ [\,g\,|\,E\,]\left[\begin{array}{c|c}1&0\\\hline 0&Q\end{array}\right] \right\|_{\mathsf{F}} = \left\| [\,g\,|\,E\,] \right\|_{\mathsf{F}}.$$

Consequently, if the original problem $Ax \approx b$ has a TLS solution, then the tilded (orthogonally transformed) problem also has a TLS solution, and there is a simple relation between them; see the following diagram:

$$\begin{tikzcd}
Ax \approx b \arrow[r, leftrightarrow] \arrow[d] & \widetilde{A}\widetilde{x} \;\equiv\; (P^{\mathsf{T}}AQ)(Q^{\mathsf{T}}x) \approx (P^{\mathsf{T}}b) \;\equiv\; \widetilde{b} \arrow[d] \\
x_{\mathsf{TLS}} \arrow[r, leftrightarrow] & \widetilde{x}_{\mathsf{TLS}} = Q^{\mathsf{T}}x_{\mathsf{TLS}}.
\end{tikzcd}$$

1.1.2 Core problem within $Ax \approx b$

Paige and Strakoš in [22] further introduced the so-called *core problem* concept. This enabled to divide the problem into two subproblems by using the orthogonal transformation above, such that the only one of them contains the relevant and all the necessary data to find the solution of the original problem.

The orthogonal transformation realized by $P \in \mathbb{O}_m$ and $Q \in \mathbb{O}_n$ applied on the original problem represented by $[b, A]$ yields the tilded problem $[\widetilde{b}, \widetilde{A}]$ in the following block form

$$\left[\ \widetilde{b} \ \middle|\ \widetilde{A}\ \right] = P^{\mathsf{T}} \left[\ b \ \middle|\ A\ \right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & Q \end{array}\right] = \left[\begin{array}{c|cc} b_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{array}\right]. \tag{1.5}$$

Here only the subproblem $A_{11}x_1 \approx b_1$ needs to be solved (as the second part $A_{22}x_2 \approx 0$ obviously has trivial solution).

Such transformation always exists (see [22]), provided the other matrix A_{22} might be degenerated (or trivial, or empty), i.e., it may have no columns, or no rows (or both). The first subproblem obtained by such transformation which has *minimal dimensions* among all suitable orthogonal transformations is called the *core problem*. The corresponding orthogonal transformation (realized by P and Q) is called the core problem revealing transformation.

The core problem $A_{11}x_1 \approx b_1$ complies with a bunch of interesting properties, namely (see [22], [11]):

$*$(CP1) The matrix $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of *full column rank* equal to $\overline{n}$.

(CP2) The vector $b_1 \in \mathbb{R}^{\overline{m}}$ is nonzero.

$*$(CP3) The scalars $u_i^{\mathsf{T}} b_1 \in \mathbb{R}$ are nonzero (where u_i are the left singular vectors of A_{11}^{T}), for $i = 1, \ldots, \overline{m}$.

(CP4) The matrix $[b_1, A_{11}] \in \mathbb{R}^{\overline{m}\times(\overline{n}+1)}$ is of *full row rank* equal to $\overline{m}$.

(CP5) The scalars $e_1^{\mathsf{T}} v_\ell \in \mathbb{R}$ are nonzero (where e_1 is the first Euclidean vector and v_ℓ are the right singular vectors of $[b_1, A_{11}]$), for $\ell = 1, \ldots, \overline{n}, \overline{n}+1$.

(CP6) Singular values of the matrix A_{11} are simple.

(CP7) Singular values of the matrix $[b_1, A_{11}]$ are simple.

Among all the properties, there are two particularly notable things. First:

The minimality of the subproblem $A_{11}x_1 \approx b_1$ is equivalent to (CP1) $\wedge$ (CP3)

see for example [4]. Another very important property is that:

The core problem $A_{11}x_1 \approx b_1$ always has the unique TLS solution $x_{1,\mathsf{TLS}}$

see [22]; in [11, Appendix A] this property is listed as (CP8).

If the original problem $Ax \approx b$ also has the unique TLS solution x_{TLS}, there is a straightforward relation between them through the transformation. See the following diagram:

$$\begin{tikzcd}
Ax \approx b \arrow[r] \arrow[d] & A_{11}x_1 \equiv (P_1^{\mathsf{T}}AQ_1)(Q_1^{\mathsf{T}}x) \approx (P_1^{\mathsf{T}}b) \equiv b_1 \arrow[d] \\
x_{\mathsf{TLS}} \arrow[r, leftrightarrow] & x_{1,\mathsf{TLS}} = Q_1^{\mathsf{T}}x_{\mathsf{TLS}}, \; x_{\mathsf{TLS}} = Q_1 \begin{bmatrix} x_{1,\mathsf{TLS}} \\ 0 \end{bmatrix}
\end{tikzcd}$$

Here

$$P = [\; P_1 \quad P_2 \;], \quad P_1 \in \mathbb{R}^{m \times \overline{m}}, \qquad Q = [\; Q_1 \quad Q_2 \;], \quad Q_1 \in \mathbb{R}^{n \times \overline{n}}.$$

Matrices P_1 and Q_1 reduce (or restrict) the original problem to the core problem within. Thus, P_1 and Q_1 represent the core problem reduction (CPR).

Since we are able to switch between $x_{1,\mathsf{TLS}}$ and x_{TLS} by using just the Q_1 matrix:

The core problem contains all the necessary and sufficient information

for solving the original problem (see also [22]); at least in the case, when the original problem has the unique TLS solution, as we have just shown. A brief discussion about the general case follows in the next section.

Finally, note that the core problem revealing transformation (P, Q) or the core problem reduction (P_1, Q_1) can be obtained by using the singular value decomposition (SVD) of the matrix A, which is useful mainly for the theoretical analysis, or computed by Golub–Kahan iterative bidiagonalization of the matrix $[b, A]$, both ways have been presented already in [22].

1.1.3 TLS solution of $Ax \approx b$ and the non-generic approach

The standard approach to the analysis of the solvability of TLS problems including results on the necessary and sufficient condition for the existence of the solution can be found in the classical paper [2]. Namely, it is shown there that for the given A and b the TLS solution may not exist, and if it does, it may not be unique. In the case of non-uniqueness, we usually want to choose one particular, typically (but not necessarily) the minimal in the 2-norm.

These issues were further developed in [30], here the authors among other things introduce the so-called non-generic approach for the problems with no TLS solution. It basically represents replacing the TLS minimization (1.2), equivalently formulated as

$$\min_{E,g} \| [\; g \mid E \;] \|_{\mathsf{F}} \qquad \text{subject to} \qquad \exists x \; : \; (A + E)x = b + g,$$

by another similar optimization problem. That is essentially the same minimization but with additional constrain

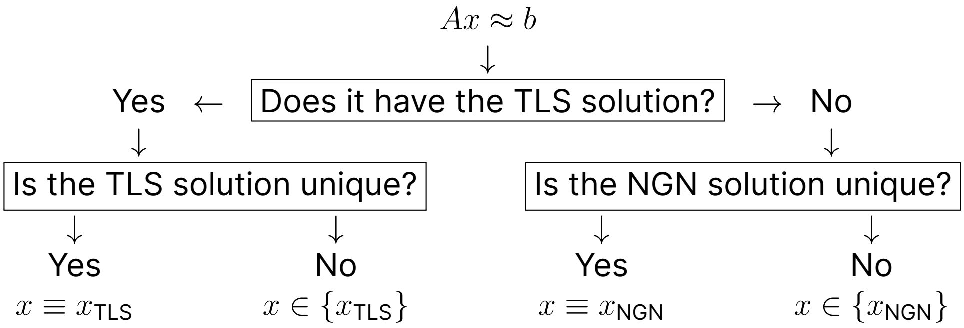
$$\min_{E,g} \| [\; g \mid E \;] \|_{\mathsf{F}} \qquad \text{subject to} \qquad \exists x \; : \; (A + E)x = b + g \; \wedge \begin{bmatrix} -1 \\ x \end{bmatrix} \perp \mathcal{V}_k,$$

where $\mathscr{V}_k$ is a span of right singular vectors of $[b, A]$ corresponding to k smallest (distinct) singular values of $[b, A]$; see [30] for details.

Note that the individual singular values may be of higher multiplicities, so $\dim(\mathscr{V}_k) \geq k$ in this formulation. Moreover, if the $(k+1)$th singular value is multiple, the above given non-generic minimization either has no solution, or it has infinitely many solutions; in the latter case we again want to choose one particular, typically (but not necessarily) the minimal in the 2-norm.

Further note that the original TLS minimization can be seen as the non-generic minimization with $k = 0$. This motivates a kind of iterative process usually called the classical TLS algorithm: In the kth step, it tries to solve the non-generic minimization with $\mathscr{V}_k$, and if there is no solution, it moves to $(k+1)$th step; see [30] or [5].

Consequently, the approximated TLS or non-generic (NGN for short) solution of $Ax \approx b$ is reached by depth-first searching the following decision-tree:



Recall that in the cases of non-uniqueness we have to decide somehow, which solution to choose.

1.1.4 Solving of $Ax \approx b$ by core problem reduction

The linear approximation problem $Ax \approx b$ can be via the core problem revealing transformation (1.5) structured such that

$$P^{\mathsf{T}} \left[\, b \,|\, A \,\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & Q \end{array}\right] = \left[\begin{array}{c|cc} b_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{array}\right].$$

Since its solvability in the TLS sense strongly relies on the properties of the SVD of $[b, A]$, the core problem concept brought some insight to it. The SVD of the whole matrix consists of the SVDs of the individual blocks of the rightmost block-diagonal matrix. Specifically, the set of singular values (including multiplicities) of $[b, A]$ is the union of such sets for $[b_1, A_{11}]$ and A_{22}. Possible TLS solvability and uniqueness of the solution then depends on the occurrence of the smallest singular value in these two blocks. In particular (see the original paper [22]):

- $\sigma_{\text{min}}(A_{22}) > \sigma_{\text{min}}([b_1, A_{11}]) \iff$ TLS solution of (1.1) exists and is unique,

- $\sigma_{\text{min}}(A_{22}) = \sigma_{\text{min}}([b_1, A_{11}]) \iff$ TLS solution of (1.1) exists, but not unique,
- $\sigma_{\text{min}}(A_{22}) < \sigma_{\text{min}}([b_1, A_{11}]) \iff$ TLS solution of (1.1) does not exist,

where σ_{min} denotes the smallest singular value of the given matrix.

Following diagrams illustrate the relations of the results when solving the TLS of the original problem, and with the use of core problem reduction with respect to four possible situations (see the decision-tree in the previous section) — there exists unique, or non-unique TLS solution, or unique or non-unique non-generic solution of the original problem.

We start with the first two cases, i.e., we assume that $Ax \approx b$ has a TLS solution, i.e.,

$$\sigma_{\text{min}}([b, A]) = \sigma_{\text{min}}([b_1, A_{11}]) \leq \sigma_{\text{min}}(A_{22})$$

(recall that CPR stands for the core problem reduction; note that these diagrams are rotated by 90° in comparison to the previous one in Section 1.1.2):

- There exists the unique TLS solution of $Ax \approx b$.

$$\begin{tikzcd} Ax \approx b \arrow[r, "\text{TLS}"] \arrow[d, "\text{CPR}"'] & x_{\text{TLS}} \arrow[d, leftrightarrow] & \text{unique} \\ A_{11}x_1 \approx b_1 \arrow[r, "\text{TLS}"] & x_{1,\text{TLS}} & \end{tikzcd}$$

- There exists a non-unique TLS solution of $Ax \approx b$.

$$\begin{tikzcd} Ax \approx b \arrow[r, "\text{TLS}"] \arrow[d, "\text{CPR}"'] & \{x_{\text{TLS}}\} & \text{non-unique} \\ A_{11}x_1 \approx b_1 \arrow[r, "\text{TLS}"] & x_{1,\text{TLS}} \arrow[u, "\text{chooses the min. } 2\text{-norm}"'] & \end{tikzcd}$$

The first diagram is already derived in Section 1.1.2, the other one follows from the properties of the core problem (in particular from a property analogous to (CP3): all right singular vectors of $[b_1, A_{11}]$ has nonzero first component); see [22]. The important thing is that the CPR chooses automatically the TLS solution minimal in the 2-norm.

If the TLS solution of $Ax \approx b$ does not exist, i.e.,

$$\sigma_{\text{min}}([b, A]) = \sigma_{\text{min}}(A_{22}) < \sigma_{\text{min}}([b_1, A_{11}]),$$

the non-generic approach is used, see [30]. We again distinguish two possibilities:

- There exists a unique non-generic solution in $AX \approx B$.

$$\begin{tikzcd} Ax \approx b \arrow[r, "\text{NGNTLS}"] \arrow[d, "\text{CPR}"'] & x_{\text{NGN}} \arrow[d, leftrightarrow] & \text{unique} \\ A_{11}x_1 \approx b_1 \arrow[r, "\text{TLS}"] & x_{1,\text{TLS}} & \end{tikzcd}$$

- There does not exist a unique non-generic solution in $Ax \approx b$.

$$\begin{tikzcd}
Ax \approx b \arrow[r, "\text{NGNTLS}"] \arrow[d, "\text{CPR}"] & \{x_{\text{NGN}}\} \quad \text{non-unique} \\
A_{11}x_1 \approx b_1 \arrow[r, "\text{TLS}"] & x_{1,\text{TLS}} \arrow[u, "\text{chooses the min. } 2\text{-norm}"']
\end{tikzcd}$$

The mechanisms here are very similar to the previous two cases. For detailed explanation we again refer to the original paper [22].

Consequently, instead of reaching the approximate TLS or NGN (minimum 2-norm) solution of $Ax \approx b$ by the decision-tree from Section 1.1.4, we can follow much simpler way

$$Ax \approx b \quad \xrightarrow{\text{CPR}} \quad A_{11}x_1 \approx b_1 \quad \xrightarrow{\text{TLS}} \quad x_{1,\text{TLS}} \quad \longrightarrow \quad x \equiv Q \begin{bmatrix} x_{1,\text{TLS}} \\ 0 \end{bmatrix}.$$

1.2 PROBLEM WITH MULTIPLE (MATRIX) RIGHT-HAND SIDE

The straightforward generalization of a single right-hand side linear approximation problem is a multiple (or matrix) right-hand side problem,

$$AX \approx B, \qquad A \in \mathbb{R}^{m \times n}, \quad B \in \mathbb{R}^{m \times d} \quad \text{such that} \quad \mathcal{R}(B) \not\subseteq \mathcal{R}(A); \qquad (1.6)$$

see [30]. It can be motivated, e.g., by the need to solve several (vector right-hand side) problems with the same system matrix, but different right-hand sides simultaneously. For instance, consider a problem with a time-dependent right-hand side

$$Ax_j \approx b_j, \quad b_j = b(t_j), \quad j = 1, 2, \ldots, d;$$

for applications see, e.g., [28], [29].

1.2.1 TLS solvability of the problem with multiple right-hand sides

The TLS minimization (1.2) can be easily generalized for problem (1.6) as

$$\min_{E,G} \| [\, E \mid G \,] \|_{\text{F}} \qquad \text{subject to} \qquad \mathcal{R}(B+E) \subseteq \mathcal{R}(A+G). \qquad (1.7)$$

The solvability analysis is even more complicated than in the single right-hand side case (and it is out of the scope of this work). The results on solvability established in classical works [2] and [30] were supplemented in [5], see also [34]. In particular, in [5] all linear approximation problems (1.6) are sorted into four classes according to their solvability properties.

This classification is based on dimensions, multiplicities of singular values of $[B, A] \in \mathbb{R}^{m\times(n+d)}$, and ranks of specific blocks of matrix V of right singular vectors of $[B, A]$. Briefly (suppose for simplicity $m \geq n + d$), let

$$[B, A] = U\Sigma V^T, \quad \text{where} \quad \Sigma = \begin{bmatrix} \mathrm{diag}(\sigma_1, \ldots, \sigma_{n+d}) \\ 0 \end{bmatrix} \in \mathbb{R}^{m\times(n+d)}, \tag{1.8}$$

be the SVD of $[B, A]$. Let numbers q $(0 \leq q \leq n)$ and e $(1 \leq e \leq d)$ denote the *left* and *right multiplicities*, respectively, of σ_{n+1}, i.e.,

$$\sigma_{n-q} > \underbrace{\sigma_{n-q+1} = \cdots = \sigma_{n+1} = \cdots = \sigma_{n+e}}_{(q+e)\text{-tuple singular value}} > \sigma_{n+e+1}. \tag{1.9}$$

Then V can be divided in the following blocks whose ranks determine the classification

$$V = \left[\begin{array}{ccc} V_{11} & V_{12} & V_{13} \\ V_{21} & V_{22} & V_{23} \\ \underbrace{\hphantom{V_{11}}}_{n-q} & \underbrace{\hphantom{V_{12}}}_{q+e} & \underbrace{\hphantom{V_{13}}}_{d-e} \end{array}\right] \begin{array}{l} \}\, d \\ \}\, n \\ \end{array} . \tag{1.10}$$

Note that if $q = n$ or $e = d$, then σ_{n-q} or σ_{n+e+1}, respectively, does not exist and matrices $\left[\begin{smallmatrix} V_{11} \\ V_{21} \end{smallmatrix}\right]$ or $\left[\begin{smallmatrix} V_{13} \\ V_{23} \end{smallmatrix}\right]$, respectively, have no columns. In particular for $d = 1$, when the matrix right-hand side problem is effectively reduced to the vector one, $e = d = 1$.

All linear approximation problems $AX \approx B$ can be now sorted into following classes:

$\mathcal{F}$ if rank$([V_{12}, V_{13}]) = d$ (the so-called *generic* problem), with three subclasses:

$\mathcal{F}_1$ if rank$(V_{12}) = e$ (and thus rank$(V_{13}) = d - e$),
$\mathcal{F}_2$ if rank$(V_{12}) > e$ and rank$(V_{13}) = d - e$, and
$\mathcal{F}_3$ if rank$(V_{13}) < d - e$ (and thus rank$(V_{12}) > e$);
note that $\mathcal{F} = \mathcal{F}_1 \cup \mathcal{F}_2 \cup \mathcal{F}_3$; and

$\mathcal{S}$ if rank$([V_{12}, V_{13}]) < d$ (the so-called *non-generic* problem).

Clearly, in the vector right-hand side case, where V_{13} has no columns (so it is always of the full column rank 0), the problems can belong only to $\mathcal{F}_1$ or $\mathcal{S}$.

In [5] it is shown that:

$$\boxed{AX \approx B \text{ has a TLS solution if and only if it belongs to } \mathcal{F}_1 \cup \mathcal{F}_2}$$

besides problems in $\mathcal{F}_3 \cup \mathcal{S}$ do not have a TLS solution. It is in particular interesting, because the classical TLS algorithm (briefly mentioned in Section 1.1.3) can be extended for the multiple right-hand side problems (see [30]), it is commonly used, and it is commonly believed, that it calculates the TLS solution for all the class $\mathcal{F}$ problems (that is why these are called generic, and the other non-generic). In [5] it is further shown, that the classical TLS algorithm moreover reaches the TLS solution only for sub-class $\mathcal{F}_1$ problems. The approximate solutions calculated for $\mathcal{F}_2$ and $\mathcal{F}_3$ problems are rather non-generic solutions. Very simple modification of the classical TLS algorithm that reaches TLS solution (at least some, not necessarily the one with minimal norm) also for sub-class $\mathcal{F}_2$ problems has been proposed in the proceedings paper [12]; see the included copy at page 35.

1.2.2 Core problem

Analogously to the single right-hand side case, orthogonal transformations of (1.6) do not change the norm in (1.7). In matrix right-hand side case it is executed by orthogonal matrices $(P, Q, R) \in \mathbb{O}_m \times \mathbb{O}_n \times \mathbb{O}_d$, such that

$$[\widetilde{B}, \widetilde{A}] = P^{\mathsf{T}}[B, A] \left[\begin{array}{cc} R & 0 \\ 0 & Q \end{array} \right] = \left[\begin{array}{cc|cc} B_1 & 0 & A_{11} & 0 \\ 0 & 0 & 0 & A_{22} \end{array} \right]. \tag{1.11}$$

The subproblem $A_{11}X_{11} = B_1$ having the minimal dimensions among all such transformations is again called the core problem, as it is introduced in [6]. It again has a lot of interesting properties, e.g.:

$*$(CP1) The matrix $A_{11} \in \mathbb{R}^{\overline{m} \times \overline{n}}$ is of *full column rank* equal to $\overline{n}$.

$*$(CP2) The matrix $B_1 \in \mathbb{R}^{\overline{m} \times \overline{d}}$ is of *full column rank* equal to $\overline{d}$.

$*$(CP3) Matrices $U_i^{\mathsf{T}} B_1 \in \mathbb{R}^{\overline{\mu}_i \times \overline{d}}$ are of *full row rank* equal to $\overline{\mu}_i$, where columns of U_i represent basis of: either the left singular subspace of A_{11} corresponding to the ith largest singular value, for $i = 1, \ldots, \overline{\xi}$; or the null-space of A_{11}^{T}, for $i = \overline{\xi} + 1$.

We particularly mention these three, because:

The minimality of subproblem $A_{11}X_{11} \approx B_1$ is equivalent to (CP1)–(CP3)

but all of the properties (CP1)–(CP7) can be generalized from the vector, to the matrix right-hand side case; see [11, Appendix A]. For example:

(CP4) The matrix $[B_1, A_{11}] \in \mathbb{R}^{\overline{m} \times (\overline{n} + \overline{d})}$ is of *full row rank* equal to $\overline{m}$.

(CP6) Multiplicities of singular values of the matrix A_{11} are bounded by $\overline{d}$.

(CP7) Multiplicities of singular values of the matrix $[B_1, A_{11}]$ are bounded by $\overline{d}$.

Most of the theoretical results are again based on the SVDs (see [6]) which is not suitable for actual computations. The generalization of the procedure for the core problem extraction based on the Golub–Kahan bidiagonalization can be found in [7].

Although the theory can be nicely generalized from the single right-hand side setting, the most interesting result related to core problems and TLS cannot be generalized. It was shown that:

$$\boxed{\textit{The core problem } A_{11}X_{11} \approx B_1 \textit{ may not have a TLS solution}}$$

the (CP8) property generalizes as: if $A_{11}X_{11} \approx B_1$ has a TLS solution, then it is unique; see [4]. This fact served as the main motivation for further research in different directions which will be covered in following parts of this thesis.

2 MOTIVATION FOR TWO DIRECTIONS OF RESEARCH

The last chapter ended with the main motivation for this whole thesis. The matrix right-hand sided core problem may not have a TLS solution. The obvious questions are: '*Why is it so?*' or more precisely: '*What does it mean, e.g., in terms of data* A *and* B *(or* A_{11} *and* B_1*)?*', '*What is wrong with the data?*' or '*Can we somehow identify such problems?*' There are two usual and very natural directions of research in such situation:

- To look inside the core problem. Try to find some potential internal structure of the core problem and study it from this perspective.
- To look at the core problems from the outside, in a wider context, i.e., look at more general settings.

Both of these ways are studied in this thesis, the '*inner view*' in Part II (see page 37; see also page 81 for the main already published results), the '*outer view*' in Part III (see page 109; see also page 139 for the main already published results).

2.1 INNER VIEW --- LOOK INSIDE THE CORE PROBLEM

Since studying the internal structure of a core problem (with matrix right-hand side) seems to be too technical in the general case, the '*reverse-engineering strategy*' can be useful, i.e., to take some existing core problems and use them as building blocks; see also Figure 2.1. This approach was already successfully applied and resulted in the so-called composed (or reducible) core problems; see [4]. Part II of this thesis formally introduces algebraic structures with which we work — including general algebraic principles and properties of composing (sets of) matrices as well as the connection to the context of linear approximation problems. Eventually, results on solvability of composed problems are presented, some parts were already published in [10] (see page 83).

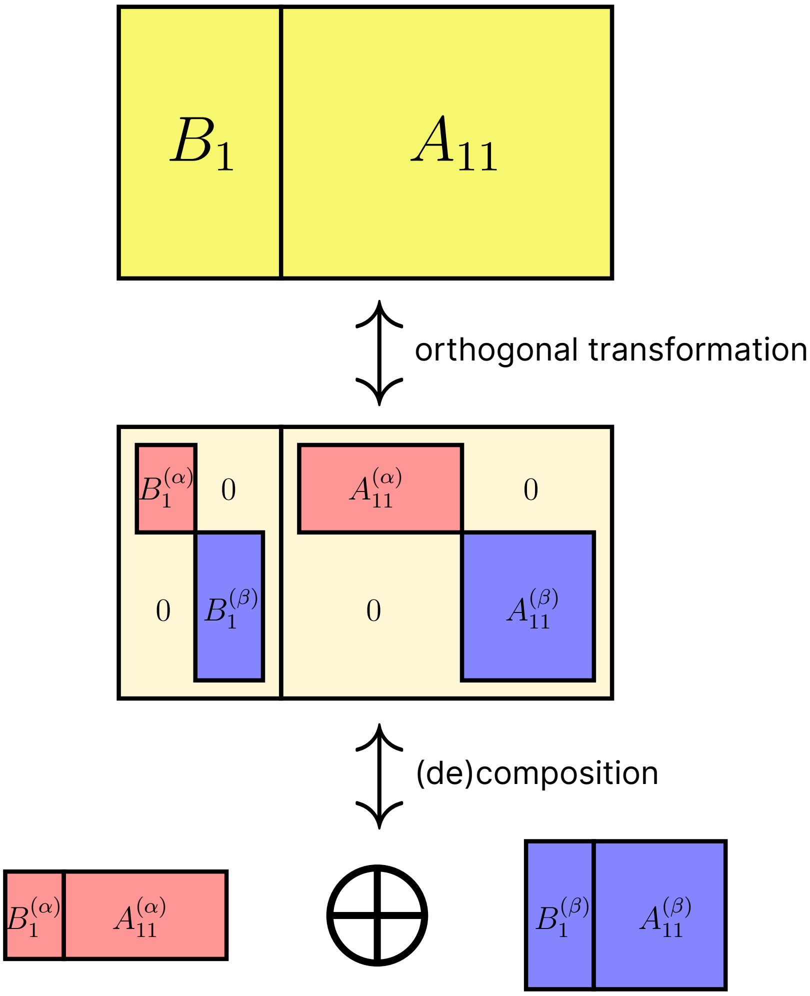


Figure 2.1: Exploring internal structure of the matrix right-hand side core problem — some core problems can be after a suitable orthogonal transformation decomposed into two (or more) fully independent core subproblems.

2.2 OUTER VIEW --- LOOK AROUND THE CORE PROBLEM

The other direction covers several ways of generalizations of the matrix case: namely the tensor right-hand side TLS problem, the bilinear TLS problem, and their unification — the general multilinear (or k-linear) TLS problems; see also Figure 2.2. This direction is covered in Part III of this thesis. All three generalizations have already been published in a series of papers, the tensor case in [8] (see page 141), the bilinear case in [9] (see page 167), and the multilinear case in [11] (see page 187).

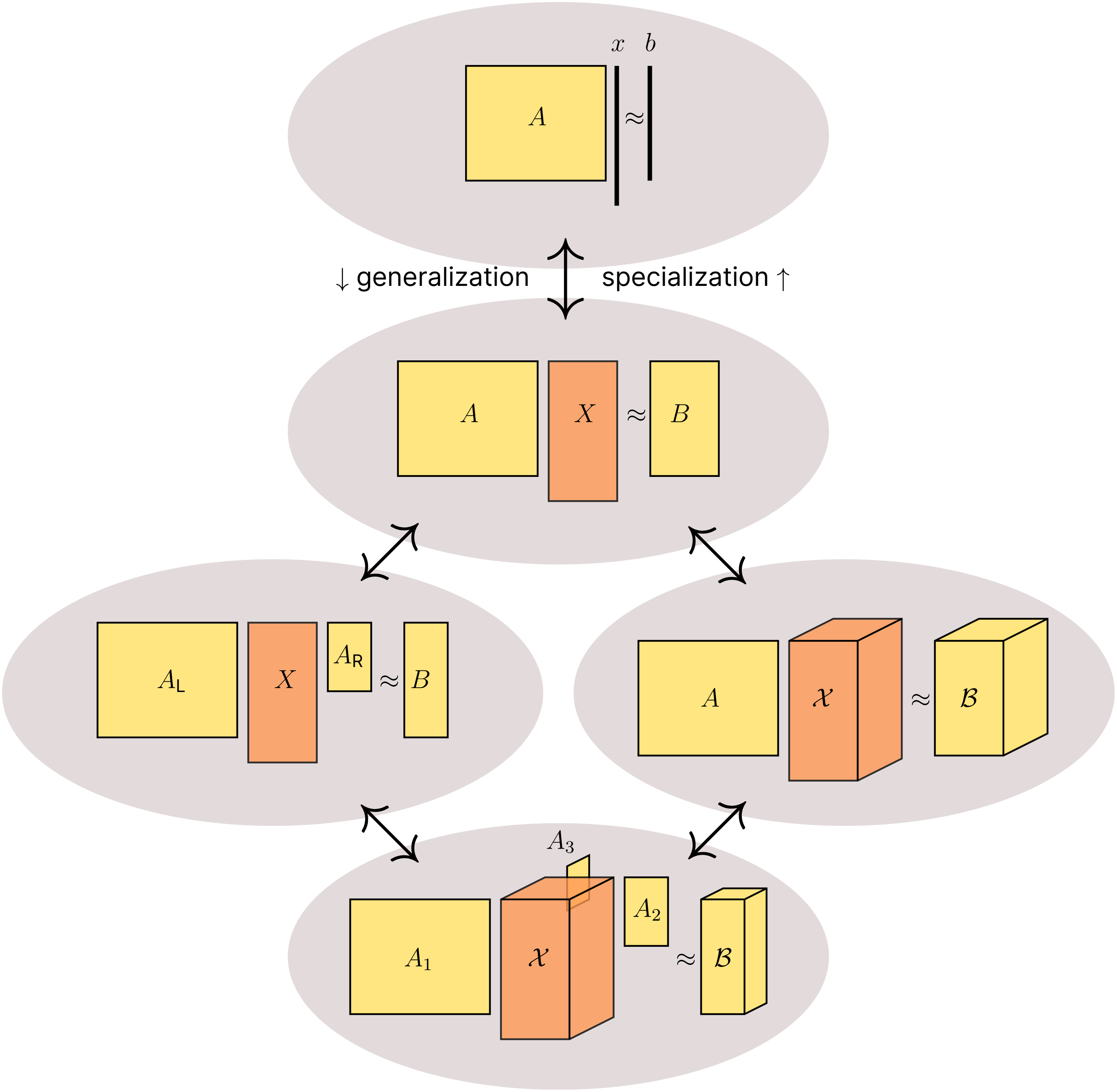


Figure 2.2: Sequence of generalizations (or specializations) of linear approximation problems: the vector right-hand side problem $Ax \approx b$ (top line), the matrix right-hand side problem $AX \approx B$ (second line), the tensor right-hand side problem $A \times_1 \mathcal{X} \approx \mathcal{B}$ (third line, right), the bilinear matrix right-hand side problem $A_\mathsf{L} X A_\mathsf{R}^\mathsf{T} \approx B$ (third line, left), and the multilinear (k-linear, here with $k = 3$) tensor right-hand side problem $(A_1, A_2, A_3 | \mathcal{X}) \approx \mathcal{B}$ (last line).

MINOR PUBLISHED RESULTS RELATED TO THE PART I

1. I. Hnětynková, M. Plešinger, and J. Žáková, *Modification of TLS algorithm for solving $\mathcal{F}_2$ linear data fitting problems*, Proceedings in Applied Mathematics and Mechanics 17 (1) (2017), pp. 749–750.

   `https://doi.org/10.1002/pamm.201710342`

   See also page 35, or reference [12].

PAMM · Proc. Appl. Math. Mech. **17**, 749 – 750 (2017) / **DOI** 10.1002/pamm.201710342

Modification of TLS algorithm for solving $\mathcal{F}_2$ linear data fitting problems

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It has been proved that the classical TLS algorithm fails to construct a TLS solution of linear data fitting problems $AX \approx B$ that belong to the class $\mathcal{F}_2$. It will be shown how to modify this algorithm in order to reach a TLS solution. Such solution is not necessarily the minimum 2-norm or Frobenius norm one. A few ideas how to decrease its norm are briefly discussed.

1 Classification of TLS problems

We are interested is solving a linear approximation problem by using the *total least squares* (TLS) minimization, i.e.,

$$AX \approx B, \quad A \in \mathbb{R}^{m\times n},\ X \in \mathbb{R}^{n\times d},\ B \in \mathbb{R}^{m\times d}, \quad \text{with} \quad m > n+d,\ \mathcal{R}(B) \not\subseteq \mathcal{R}(A),\ A^T B \neq 0, \tag{1}$$

$$\min \|[G, E]\|_F \quad \text{subject to} \quad \mathcal{R}(B+G) \subseteq \mathcal{R}(A+E). \tag{2}$$

Any matrix X_{TLS} satisfying $(A+E)X_{\mathrm{TLS}} = B+G$ for the minimizer $[G, E]$ is called the TLS solution. Analysis of such problems can be based on the (economic) singular value decomposition (SVD)

$$[B, A] = U\Sigma V^T, \quad U \in \mathbb{R}^{m\times(n+d)}, \quad \Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{n+d}),\ V \in \mathbb{R}^{(n+d)\times(n+d)};$$

see [1–3, 6–8], see also [4, 5]. Let z be the number of *distinct* singular values of $[B, A]$. Denote their multiplicities by m_t, $t = 1, \ldots, z$. Let σ_{n+1} be the kth largest singular value with the multiplicity $m_k = q + e$ so that $\sigma_{n-q} > \sigma_{n-q+1} = \cdots = \sigma_{n+1} = \cdots = \sigma_{n+e} > \sigma_{n+e+1}$. According to [3], consider the following notation of sub-matrices and sub-columns of $V \in \mathbb{R}^{(n+d)\times(n+d)}$,

$$V = \begin{bmatrix} V_{11} & V_{12} & V_{13} \\ V_{21} & V_{22} & V_{23} \end{bmatrix} = \begin{bmatrix} V'_{1,1} & \cdots & V'_{1,z} \\ V'_{2,1} & \cdots & V'_{2,z} \end{bmatrix} = \begin{bmatrix} v_{1,1} & \cdots & v_{1,n+d} \\ v_{2,1} & \cdots & v_{2,n+d} \end{bmatrix} \begin{matrix} \}\ d \\ \}\ n \end{matrix}, \tag{3}$$

where $V_{11} \in \mathbb{R}^{d\times(n-q)}$, $V_{12} \in \mathbb{R}^{d\times(q+e)}$, $V_{13} \in \mathbb{R}^{d\times(d-e)}$; $V'_{1,t} \in \mathbb{R}^{d\times m_t}$, $t = 1, \ldots, z$; and $v_{1,j} \in \mathbb{R}^d$, $j = 1, \ldots, n+d$. Thus in particular $V_{12} = V'_{1,k} = [v_{1,n-q+1}, \ldots, v_{1,n+e}]$ is the sub-block corresponding to σ_{n+1}.

Analysis in [3] divides problems (1) into several classes based on the properties of the blocks in (3). If $\mathrm{rank}([V_{12}, V_{13}]) = d$, then (1) belongs to the set $\mathcal{F}$ (corresponding to generic problems in [6]). Otherwise it belongs to the set $\mathcal{S}$ (nongeneric problems in [6]). The set $\mathcal{F}$ is futher divided into three mutually disjoint subsets, $\mathcal{F} = \mathcal{F}_1 \cup \mathcal{F}_2 \cup \mathcal{F}_3$, where:

- If $\mathrm{rank}(V_{12}) = e \wedge \mathrm{rank}(V_{13}) = d - e$, then (1) belongs to $\mathcal{F}_1$;
- if $\mathrm{rank}(V_{12}) > e \wedge \mathrm{rank}(V_{13}) = d - e$, then (1) belongs to $\mathcal{F}_2$;
- if $\mathrm{rank}(V_{12}) > e \wedge \mathrm{rank}(V_{13}) < d - e$, then (1) belongs to $\mathcal{F}_3$.

The problem (1) has a TLS solution *if and only if* it belongs to $\mathcal{F}_1 \cup \mathcal{F}_2$, i.e. $\mathrm{rank}([V_{12}, V_{13}]) = d \wedge \mathrm{rank}(V_{13}) = d - e$. The minimum Frobenius and 2-norm TLS solution of $\mathcal{F}_1$-problem takes the well-know closed-form

$$X_{\mathrm{TLS}} = -[V_{22}, V_{23}][V_{12}, V_{13}]^{\dagger}, \tag{4}$$

where † denotes the Moore–Penrose pseudoinverse. However, this is not true for the $\mathcal{F}_2$-problems; see [3]. Note that for problems in $\mathcal{F}_3$ and $\mathcal{S}$ the TLS solution does not exist.

2 Modification of the TLS algorithm

The problem (2) is typically solved by the *classical TLS algorithm* (see [6, pp. 87–88], [3, p. 767]). This algorithm seeks for the largest ℓ so that $\mathrm{rank}([V'_{1,\ell}, \ldots, V'_{1,z}]) = d$, and gives the output approximation in the form

$$X_{\mathrm{OUT}} = -[V'_{2,\ell}, \ldots, V'_{2,z}][V'_{1,\ell}, \ldots, V'_{1,z}]^{\dagger}. \tag{5}$$

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If (1) belongs to $\mathcal{F}$, then $[V_{12}, V_{13}] = [V'_{1,k}, \ldots, V'_{1,z}]$ is of rank d, whereas rank of $V_{13} = [V'_{1,k+1}, \ldots, V'_{1,z}] \in \mathbb{R}^{d\times(d-e)}$, $e \geq 1$, is always smaller. Thus $\ell = k$ and the right-hand sides of (4) and (5) coincide. However, (5) represents a TLS solutions only for $\mathcal{F}_1$-problems, since a TLS solution of $\mathcal{F}_2$-problems can not be expressed in this form; see [3]. Here (5) can be understood only as a *nongeneric-like solution* of (2). For $\mathcal{S}$-problems, $[V_{12}, V_{13}]$ is always rank-deficient and thus $\ell < k$.

These results reveal that it is necessary to modify the TLS algorithm in order to construct a TLS solution for $\mathcal{F}_2$-problems. Based on [3], determination of a TLS solution requires to find an orthogonal matrix in the *orthogonal group* $\mathbb{O}(s) = \{Q \in \mathbb{R}^{s\times s} : Q^T = Q^{-1}\}$, $s = q + e$, such that $[V_{12}Q, V_{13}][0, I_d]^T \in \mathbb{R}^{d\times d}$ is invertible. Then the matrix

$$X_{\mathrm{TLS}} = -[V_{22}Q, V_{23}] \begin{bmatrix} 0 \\ I_d \end{bmatrix} \left([V_{12}Q, V_{13}] \begin{bmatrix} 0 \\ I_d \end{bmatrix} \right)^{-1} \tag{6}$$

represents the corresponding TLS solution. Denote $Q^{[F]}$ and $Q^{[2]}$ the matrices corresponding to the minimum Frobenius and 2-norm TLS solution, respectively. For $\mathcal{F}_1$-problems, $Q^{[F]} = Q^{[2]}$ and this matrix can be obtained explicitly by a (left-right-reordered) LQ decomposition of V_{12}, or implicitely by the Moore–Penrose pseudoinverse of $[V_{12}, V_{13}]$ in (4). However, for $\mathcal{F}_2$-problems $Q^{[F]}$ and $Q^{[2]}$ may be different. Their determination would require searching at least the whole *special orthogonal group* $\mathbb{SO}(s)$ defined as the largest connected subgroup of $\mathbb{O}(s)$ (since (6) is independent on the sign of $\det(Q)$); see [3]. This is for larger s computationally unfeasible. In order to construct some (not necessarily minimum norm) TLS solution, we reduce the search set. First, we replace $\mathbb{O}(s)$ by its subgroup of permutation matrices $\mathbb{P}(s) = \{\Pi \in \{0,1\}^{s\times s}, \Pi^T = \Pi^{-1}\}$, i.e., the smooth minimization is replaced by a discrete minimization of the size $s!$ with $s = q + e$. Now we are able to construct a TLS solution. For the $\mathcal{F}_2$-problem, there always exist e columns of V_{12} such that

$$[V_{12}\Pi, V_{13}] \begin{bmatrix} 0 \\ I_d \end{bmatrix} = \Big[[v_{1,n-q+\pi(q+1)}, \ldots, v_{1,n-q+\pi(q+e)}], V_{13} \Big] \in \mathbb{R}^{d\times d} \tag{7}$$

is invertible, where the permutation $\pi(\cdot)$ (realized by Π), selects the above mentioned e columns. Clearly, this selection is done only among columns satisfying $v_{1,n-q+j} \notin \mathcal{R}(V_{13})$, $j = 1, \ldots, q + e$, which simplifies the discrete minimization. The modified TLS algorithm is then given in Algorithm 1.

Algorithm 1 $\mathcal{F}_2$-adaptation of the TLS algorithm

```
00  Input $A, B, m, n, d$; compute SVD $[B, A] = U\Sigma V^T$ and identify $q, e, V_{\alpha\beta}, m_t, k, z, V'_{i,t}$
01  If $\mathrm{rank}([V_{12}, V_{13}]) = d$ then problem is of first class ($\mathcal{F}$), also called generic problem
02    If $\mathrm{rank}(V_{13}) = e$ and $\mathrm{rank}(V_{12}) = d - e$ then problem is of class $\mathcal{F}_1$
03      Output $X_{\mathrm{OUT}} = X_{\mathrm{TLS}} = -[V_{22}, V_{23}][V_{12}, V_{13}]^\dagger$, the minimum Frob. and 2-norm TLS solution
04    elseif $\mathrm{rank}(V_{13}) = e$ and $\mathrm{rank}(V_{12}) > d - e$ then problem is of class $\mathcal{F}_2$
05      Find the set of all columns of $V_{12}$ satisfying $v_{1,n-q+j} = V_{12}e_j \notin \mathcal{R}(V_{13})$
06      Select some subset of $e$ of them—let it contains the $j_1$th, $j_2$th, ..., and $j_e$th columns of $V_{12}$
07      Find a permutation matrix $\Pi$ so that $V_{12}\Pi = [\ldots, v_{1,n-q+j_1}, v_{1,n-q+j_2}, \ldots, v_{1,n-q+j_e}]$
08      Output $X_{\mathrm{F2\text{-}OUT}} = X_{\mathrm{TLS}} = -([V_{22}\Pi, V_{23}][\begin{smallmatrix} 0 \\ I_d \end{smallmatrix}])([V_{12}\Pi, V_{13}][\begin{smallmatrix} 0 \\ I_d \end{smallmatrix}])^{-1}$, some TLS solution
09    elseif $\mathrm{rank}(V_{13}) < e$ then problem is of class $\mathcal{F}_3$
10      Output $X_{\mathrm{OUT}} = -[V_{22}, V_{23}][V_{12}, V_{13}]^\dagger$, the nongeneric-like solution
11  elseif $\mathrm{rank}([V_{12}, V_{13}]) < d$ then problem is of second class ($\mathcal{S}$), also called nongeneric problem
12    Find $\ell$ ($\ell < k$) so that $\mathrm{rank}([V'_{1,\ell}, \ldots, V'_{1,z}]) = d$ and $\mathrm{rank}([V'_{1,\ell+1}, \ldots, V'_{1,z}]) < d$
13    Output $X_{\mathrm{OUT}} = -[V'_{2,\ell}, \ldots, V'_{2,z}][V'_{1,\ell}, \ldots, V'_{1,z}]^\dagger$, the so-called nongeneric solution
```

In the original TLS algorithm, a single line **Output** $X_{\mathrm{OUT}} = -[V_{22}, V_{23}][V_{12}, V_{13}]^\dagger$ substitutes the lines `02`–`10`.

To get a TLS solution reasonably close to the minimum norm solution, the selection of e columns in the line `06` needs to be specified. Here we can employ ideas used originally, e.g., in the proof of Theorem 3.6 in [6], or in Section 3.4 of [3]. The selection needs to maximize the Frobenius norm of the invertible matrix (7) and at the same time keep it enough far from being singular. Thus we have to focus on columns $v_{1,n-q+j}$ with larger norms and smaller inner products among themselves, and with the columns of V_{13}. Further study is however out of the scope of this contribution.

Acknowledgements This work was supported by the project 17-04150J funded by the Grant Agency of the Czech Republic.

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PART II

INNER STRUCTURE OF MATRIX RIGHT-HAND SIDE CORE PROBLEMS

3 SELECTED BASIC ALGEBRAIC STRUCTURES PRESENT IN THE SET OF ALL MATRICES

In this chapter we aim to review some basic algebraic structures that are present in the set of all matrices and introduce corresponding notation. That would allow us to further introduce some kind of arithmetics based on the direct sum, which will be useful (in the next Chapter 4) for the description of the inner structure of linear approximation problem and core problems specifically.

3.1 VECTORS SPACES, GROUPS, AND OTHER SETS OF MATRICES

First, we briefly remind some of the very basic concepts. We do it in particular because we need to carefully include the trivial cases — matrices with no columns or rows; see the discussion below (1.5). Therefore, we start by denoting

$$\mathbb{N} = \{1, 2, 3, \ldots\} \quad \text{and} \quad \mathbb{N}_0 = \mathbb{N} \cup \{0\}$$

the sets of all *positive* and *nonnegative integers*, respectively.

In the text we deal in general with m-by-k matrices with entries from some given set $\mathbb{S}$. The set of all such matrices is denoted as usual by $\mathbb{S}^{m\times k}$. In order to do some reasonable arithmetics with such matrices, $\mathbb{S}$ use to be an underlying set of some *algebraic ring*, at least. If $\mathbb{S}$ is an underlying set of some *algebraic field*, let say $\mathbb{F}$, then $\mathbb{F}^{m\times k}$ forms the *linear vector space* over this field.

In the introductory Part I, we always consider real matrices, so there is $\mathbb{F} = \mathbb{R}$ — the *field of real numbers* (*reals* for short). However, it is worth to note here that all the theory there can be straightforwardly reformulated for complex matrices and vectors, and for complex linear approximation problems. The same would be true in the rest of the text. More specifically, we mostly consider $\mathbb{R}$, and possible extensions to *complex numbers* $\mathbb{C}$ are commented; other underlying sets $\mathbb{S}$ or algebraic fields $\mathbb{F}$ different from $\mathbb{R}$ or $\mathbb{C}$ are not appropriate, and thus not considered in this text.

3.1.1 Vector spaces of empty matrices

Vector spaces of real matrices $\mathbb{R}^{m\times k}$ are usually considered such that $m, k \in \mathbb{N}$; note that the zero matrix (the neutral element w.r.t. summation in $\mathbb{R}^{m\times k}$) we denote by $0_{m,k}$. As already suggested, it will be useful for us to deal also with matrices with zero number of rows or columns, i.e., we allow $m, k \in \mathbb{N}_0$. In other words, we also consider an infinitely many *degenerated* (or *trivial*) vector spaces, each containing only one neutral element — the *empty matrix* — and the zero matrix at the same time,

$$\mathbb{R}^{m\times 0} = \{0_{m,0}\}, \quad 0_{m,0} = \begin{bmatrix} \\ \\ \\ \end{bmatrix}, \qquad \mathbb{R}^{0\times k} = \{0_{0,k}\}, \quad 0_{0,k} = [\qquad\qquad\quad]. \tag{3.1}$$

Among these degenerated spaces

$$\mathbb{R}^{0\times 0} = \{0_{0,0}\}, \qquad 0_{0,0} = [\,] \tag{3.2}$$

is particularly important.

Note here that we often write the zero matrix simply by 0, i.e., without specification of its dimensions. We specify them only if it is necessary for understanding, or if the matrix is empty.

3.1.2 Arithmetics of empty matrices

The standard matrix arithmetics can be straightforwardly extended to the empty matrices. In particular, for $M \in \mathbb{R}^{m\times k}$,

$$M0_{k,0} = 0_{m,0}, \quad 0_{0,m}M = 0_{0,k}, \quad 0_{0,s}0_{s,0} = 0_{0,0}, \quad 0_{m,0}0_{0,k} = 0_{m,k}, \tag{3.3}$$

where $0_{m,k} \in \mathbb{R}^{m\times k}$ is the m-by-k *zero matrix*.

Furthermore, matrix $M \in \mathbb{R}^{m\times k}$ trivially cannot be changed neither by *concatenation* with an empty matrix of suitable dimensions

$$[M, 0_{m,0}] = \begin{bmatrix} M \\ 0_{0,k} \end{bmatrix} = M = \begin{bmatrix} 0_{0,k} \\ M \end{bmatrix} = [0_{m,0}, M] \tag{3.4}$$

and thus nor by the *block-diagonal composition* (first and last case) and *block-antidiagonal composition* (middle cases),

$$\underbrace{\begin{bmatrix} M & \\ & 0_{0,0} \end{bmatrix}}_{\text{diag}(M,\, 0_{0,0})} = \begin{bmatrix} & M \\ 0_{0,0} & \end{bmatrix} = M = \begin{bmatrix} & 0_{0,0} \\ M & \end{bmatrix} = \underbrace{\begin{bmatrix} 0_{0,0} & \\ & M \end{bmatrix}}_{\text{diag}(0_{0,0},\, M)}. \tag{3.5}$$

Note that the block-diagonal composition is often called the *direct sum* of matrices.

3.1.3 $\mathscr{M}$: The set of all matrices

The title of this chapter mentions *the set of all matrices*. By this we refer to the set

$$\mathscr{M} \equiv \mathscr{M}(\mathbb{R}) \equiv \bigcup_{m,k\in\mathbb{N}_0} \mathbb{R}^{m\times k}, \tag{3.6}$$

i.e., the set of all real matrices, including empty matrices. Similarly $\mathscr{M}(\mathbb{C})$, $\mathscr{M}(\mathbb{F})$, and $\mathscr{M}(\mathbb{S})$ denote sets of all complex matrices, matrices over field $\mathbb{F}$, and set $\mathbb{S}$, respectively.

3.1.4 Groups of orthogonal (and unitary) matrices

Further, we will require to work with a special sort of *square invertible matrices* called the *orthogonal matrices*; see (1.4). Recall that

$$P \in \mathbb{R}^{m\times m} \text{ is orthogonal} \qquad \Longleftrightarrow \qquad P^{-1} = P^{\mathsf{T}}, \tag{3.7}$$

or, equivalently, $PP^{\mathsf{T}} = I_m = P^{\mathsf{T}}P$. Just to be sure, here P^{T} denotes the matrix *transposed* to P and I_m stands for the m-by-m *identity matrix*. Note that in the case of complex field (and that is one of changes that we need to implement when translating Part I to complex numbers) we need to deal with the so-called *unitary matrices*,

$$P \in \mathbb{C}^{m\times m} \text{ is unitary} \qquad \Longleftrightarrow \qquad P^{-1} = P^{\mathsf{H}}, \tag{3.8}$$

or, equivalently, $PP^{\mathsf{H}} = I_m = P^{\mathsf{H}}P$. Here $P^{\mathsf{H}} = (\overline{P})^{\mathsf{T}} = \overline{(P^{\mathsf{T}})}$ denotes the *complex conjugate transposition* (bars denote the complex conjugation).

The sets of all orthogonal and unitary matrices of the given fixed size m, denoted usually

$$\mathbb{O}_m \subseteq \mathbb{R}^{m\times m} \qquad \text{and} \qquad \mathbb{U}_m \subseteq \mathbb{C}^{m\times m},$$

form together with the matrix multiplication the so-called *orthogonal* and *unitary groups*, respectively. If the size of the orthogonal, or unitary matrix P is not specified, we write simply $P \in \mathbb{O}$, or $P \in \mathbb{U}$, respectively.

In the case $m = 0$, we consider

$$\mathbb{O}_0 = \mathbb{U}_0 = \mathbb{R}^{0\times 0} = \{0_{0,0}\}.$$

This might be a bit disturbing to the reader, because the empty matrix $0_{0,0}$ is the zero of the vector space $\mathbb{F}^{0\times 0}$, but it plays also the role of the neutral element within the multiplicative group. But it is perfectly fine because the identity matrix I_m with $m = 0$, i.e., of order zero, satisfies $I_0 = 0_{0,0}$. (Note this situation is analogous to algebraic rings, where the zero 0 and the unit 1 elements are the same $0 = 1$. Such so-called zero-rings contain only one element.) Now it would be no surprise, that we consider

$$\text{det}(0_{0,0}) = 1$$

for convenience.

3.2 DIRECT SUMMATION MONOID $(\mathscr{M}, \oplus)$

The *direct sum* of two matrices (or the *block-diagonal composition*, as already mentioned) is defined as

$$M_1 \oplus M_2 \equiv \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} = M \in \mathbb{R}^{m \times k}, \tag{3.9}$$

where $M_j \in \mathbb{R}^{m_j \times k_j}$, $j = 1, 2$, $M \in \mathbb{R}^{m \times k}$, and $m = m_1 + m_2$, $k = k_1 + k_2$.

One can see that the direct sum $\oplus$ is a *binary operation* on the set $\mathscr{M}$ satisfying a lot of obvious and useful properties:

(S1) Trivially, the set $\mathscr{M}$ is *closed* w.r.t. $\oplus$ (which is, in fact, already hidden in the term *operation*), i.e.,

$$\oplus \; : \; \mathscr{M}^2 \longrightarrow \mathscr{M}.$$

(S2) The direct sum is *associative*, i.e.,

$$\forall M_1, M_2, M_3 \in \mathscr{M}, \quad (M_1 \oplus M_2) \oplus M_3 = M_1 \oplus (M_2 \oplus M_3)$$

that allows us to write simply $M_1 \oplus M_2 \oplus M_3$.

(S3) There is a *neutral element* w.r.t. $\oplus$ within $\mathscr{M}$ (see (3.5)), i.e.,

$$\exists 0_{0,0} \in \mathscr{M}, \quad \forall M \in \mathscr{M}, \quad M \oplus 0_{0,0} = M = 0_{0,0} \oplus M.$$

(S4) The direct sum is clearly *not commutative* up to some special cases. For example if at least one of these cases occurs:

- $M_1 = M_2$,
- $M_1 = 0_{0,0}$,
- $M_2 = 0_{0,0}$,
- $M_1 = 0_{m_1,k_1}$ and $M_2 = 0_{m_2,k_2}$,

then $M_1 \oplus M_2 = M_2 \oplus M_1$.

Consequently, $\mathscr{M}$ together with $\oplus$ form an algebraic structure specified in the following proposition that we have just proved:

Proposition 1. *Let $\mathscr{M}$ be the set of all matrices over the real numbers (3.6) and let $\oplus : \mathscr{M}^2 \longrightarrow \mathscr{M}$ be the direct summation defined on $\mathscr{M}$ by (3.9). Then the ordered pair*

$$(\mathscr{M}, \oplus)$$

forms the structure of non-commutative monoid.

3.2.1 Direct summation and empty matrices

Let us also mention that the admission of having the matrix with the zero number of columns or rows enables us to introduce following identities extending the neutrality property (S3). Having $M_1 \in \mathbb{R}^{m_1 \times k_1}$ and M_2 being an empty matrix, in particular $M_2 \equiv 0_{m_2,0} \in \mathbb{R}^{m_2 \times 0}$, the direct sum takes the form

$$M_1 \oplus M_2 = M_1 \oplus 0_{m_2,0} = \underbrace{\begin{bmatrix} M_1 \\ 0_{m_2,k_1} \end{bmatrix}}_{k_1} \begin{matrix} \}\, m_1 \\ \}\, m_2 \end{matrix}\,, \tag{3.10}$$

in the other case $M_2 \equiv 0_{0,k_2} \in \mathbb{R}^{0 \times k_2}$

$$M_1 \oplus M_2 = M_1 \oplus 0_{0,k_2} = \big[\, \underbrace{M_1}_{k_1} \;\; \underbrace{0_{m_1,k_2}}_{k_2} \,\big] \} m_1. \tag{3.11}$$

Similarly it behaves when M_1 is an empty and M_2 a general matrix.

Combining the previous two identities together with the associativity (S2), we see

$$\forall M_1 \in \mathscr{M}, \quad (M_1 \oplus 0_{m_2,0}) \oplus 0_{0,k_2} = M_1 \oplus (0_{m_2,0} \oplus 0_{0,k_2}) = M_1 \oplus 0_{m_2,k_2},$$

consequently giving

$$0_{m_2,0} \oplus 0_{0,k_2} = 0_{m_2,k_2} = 0_{m_2,0}\, 0_{0,k_2} = 0_{0,k_2} \oplus 0_{m_2,0}; \tag{3.12}$$

see also (3.3) for the second and (S4) for the third equality. Finally note that

$$0_{m_1,0} \oplus 0_{m_2,0} = 0_{m_1+m_2,0} \qquad \text{and} \qquad 0_{0,k_1} \oplus 0_{0,k_2} = 0_{0,k_1+k_2}. \tag{3.13}$$

3.2.2 Direct sum of subsets of $\mathscr{M}$

The direct sum can be simply generalized so that it performs on the whole sets. Suppose $\mathscr{M}_1$, $\mathscr{M}_2 \subseteq \mathscr{M}$ are nonempty. Then we can define the direct sum

$$\mathscr{M}_1 \oplus \mathscr{M}_2 = \{M_1 \oplus M_2 \;:\; M_1 \in \mathscr{M}_1,\; M_2 \in \mathscr{M}_2\} \subseteq \mathscr{M}. \tag{3.14}$$

Apparently,

$$\mathscr{M} \oplus \mathscr{M} \subseteq \mathscr{M},$$

i.e., the set $\mathscr{M}$ is closed w.r.t. the direct sum; see (S1). Furthermore, since the empty matrices are within $\mathscr{M}$, it is easy to show that

$$\mathscr{M} \oplus \mathscr{M} = \mathscr{M}. \tag{3.15}$$

It trivially comes out from the fact that

$$\forall M \in \mathscr{M}, \quad \exists M_1, M_2 \in \mathscr{M}, \quad M = M_1 \oplus M_2 \tag{3.16}$$

complemented with the fact that the matrix $0_{0,0} \in \mathbb{R}^{0 \times 0}$ plays the role of the neutral element w.r.t. $\oplus$; see property (S3). To show (3.16) we can take $M_1 = M$, $M_2 = 0_{0,0}$, or vice versa.

3.3 ORTHOGONAL EQUIVALENCE & QUOTIENT SET $\mathscr{M}/_{\sim}$

Consider two matrices of the same dimension M, $L \in \mathbb{R}^{m\times k} \subset \mathscr{M}$. The following definition introduces an *equivalence relation* on the set $\mathscr{M}$.

Definition 1 (orthogonal equivalence)**.** *We say that L is orthogonally equivalent to M, if there exist orthogonal matrices $P \in \mathbb{O}_m$ and $S \in \mathbb{O}_k$ such that*

$$L = P^{\mathsf{T}} M S, \tag{3.17}$$

shortly $L \sim M$.

It is easy to verify that this relation really is an equivalence. It clearly satisfies the following properties:

$\forall K, L, M \in \mathscr{M}$,

$$\begin{aligned} &\text{(reflexivity)} && M = I^{\mathsf{T}} M I \sim M, \\ &\text{(symmetry)} && L = P^{\mathsf{T}} M S \sim M \iff M = PLS^{\mathsf{T}} = (P^{\mathsf{T}})^{\mathsf{T}} L (S^{\mathsf{T}}) \sim L, \\ &\text{(transitivity)} && K = P_1^{\mathsf{T}} L S_1 \sim L \;\&\; L = P_2^{\mathsf{T}} M S_2 \sim M \implies \\ &&& K = P_1^{\mathsf{T}} (P_2^{\mathsf{T}} M S_2) S_1 = (P_2 P_1)^{\mathsf{T}} M (S_2 S_1) \sim M, \end{aligned}$$

since the set of orthogonal matrices of the given order together with matrix multiplication form a group.

3.3.1 Equivalence classes

Using this equivalence relation, we can establish equivalence classes in a standard way such that

$$[M]_{\sim} = \{ L \in \mathscr{M} \;:\; L \sim M \}. \tag{3.18}$$

Clearly, since the equivalence is defined with the use of a multiplication by square matrices, if $M \in \mathbb{R}^{m\times k}$, then $[M]_{\sim} \subseteq \mathbb{R}^{m\times k}$.

Remark 1. *Employing the singular value decomposition (SVD), we can express M as the product of a diagonal matrix Σ and two orthogonal matrices $U \in \mathbb{O}_m$ and $V \in \mathbb{O}_k$ such that*

$$M = U\Sigma V^{\mathsf{T}}, \qquad \text{i.e.,} \qquad \Sigma = U^{\mathsf{T}} M V. \tag{3.19}$$

We see that $\Sigma \sim M$, and thus we can take Σ as the natural representative of the class $[M]_{\sim}$.

In other words, any equivalence class $[M]_{\sim}$, $M \in \mathbb{R}^{m\times k} \subset \mathscr{M}$, is uniquely given by the dimensions and singular values of M, i.e., by the triplet

$$\Big(m, k, \big[\sigma_1(M), \sigma_2(M), \ldots, \sigma_{\min(m,k)}(M) \big] \Big),$$

where $\sigma_j(M)$ denotes the jth largest singular value of M.

3.3.2 Classes of empty & zero matrices

Since each of the degenerated spaces always consists of the only (empty) matrix, the corresponding class also contains the only matrix, i.e.,

$$[0_{0,0}]_\sim = \{0_{0,0}\} = \mathbb{R}^{0\times 0}, \quad [0_{m,0}]_\sim = \{0_{m,0}\} = \mathbb{R}^{m\times 0}, \quad [0_{0,k}]_\sim = \{0_{0,k}\} = \mathbb{R}^{0\times k}.$$

Further, the classes corresponding to nonempty, but zero matrices

$$[0_{m,k}]_\sim = \left\{P0_{m,k}S^\mathsf{T} = 0_{m,k} \;:\; P \in \mathbb{O}_m,\, S \in \mathbb{O}_k\right\} = \{0_{m,k}\} \subseteq \mathbb{R}^{m\times k}$$

always contain the only matrix as well.

3.3.3 Quotient set

Consequently, $\mathscr{M}$ can be decomposed into mutually disjoint classes of equivalence yielding a *quotient set*

$$\mathscr{M}/_\sim = \left\{[M]_\sim \;:\; M \in \mathscr{M}\right\}. \tag{3.20}$$

Since the set of singular values of the direct sum is the union of sets of singular values of individual summands, we can combine both concepts together. It allows us to modify the binary operation — the direct sum — for the quotient set; and then form the quotient monoid.

3.4 QUOTIENT MONOID $(\mathscr{M}/_\sim, \boxplus)$

The binary operation on the quotient set $\mathscr{M}/_\sim$ dealing with the (representatives of) equivalence classes can be defined as

$$[M_1]_\sim \boxplus [M_2]_\sim = [M_1 \oplus M_2]_\sim\,. \tag{3.21}$$

Similarly as before, this operation has a lot of important properties:

($\widetilde{\text{S}}$1) Again, the set $\mathscr{M}/_\sim$ is clearly *closed* w.r.t. $\boxplus$, i.e.,

$$\boxplus \;:\; (\mathscr{M}/_\sim)^2 \longrightarrow \mathscr{M}/_\sim\,.$$

($\widetilde{\text{S}}$2) The operation $\boxplus$ is *associative*, i.e., $\forall [M_1]_\sim, [M_2]_\sim, [M_3]_\sim \in \mathscr{M}/_\sim$

$$\begin{aligned}\Big([M_1]_\sim \boxplus [M_2]_\sim\Big) \boxplus [M_3]_\sim &= [M_1 \oplus M_2]_\sim \boxplus [M_3]_\sim \\ &= [(M_1 \oplus M_2) \oplus M_3]_\sim = [M_1 \oplus (M_2 \oplus M_3)]_\sim \\ &= [M_1]_\sim \boxplus [M_2 \oplus M_3]_\sim = [M_1]_\sim \boxplus \Big([M_2]_\sim \boxplus [M_3]_\sim\Big)\end{aligned}$$

that allows us to write simply $[M_1]_\sim \boxplus [M_2]_\sim \boxplus [M_3]_\sim$.

($\widetilde{\text{S}}$3) There is a *neutral element* $[0_{0,0}]_\sim$ within $\mathscr{M}/_\sim$, i.e.,

$$\forall [M]_\sim \in \mathscr{M}/_\sim, \quad [M]_\sim \boxplus [0_{0,0}]_\sim = [M \oplus 0_{0,0}]_\sim = [M]_\sim,$$

and similarly from the other side.

($\widetilde{\text{S}}$4) Contrary to $\oplus$, the operation $\boxplus$ is *commutative*.

To show the commutativity consider first, for the given fixed splitting $n = n_1 + n_2$, the following bijection f_{n_1,n_2} on $\mathbb{R}^{n\times n}$

$$f_{n_1,n_2} \,:\, G \longmapsto f_{n_1,n_2}(G) = \begin{bmatrix} 0 & I_{n_2} \\ I_{n_1} & 0 \end{bmatrix} G, \qquad f^{-1}_{n_1,n_2} = f_{n_2,n_1}.$$

Clearly, for $m = m_1 + m_2$, $P \in \mathbb{O}_m$ if and only if $f_{m_1,m_2}(P) \in \mathbb{O}_m$; and similarly for $k = k_1 + k_2$, $S \in \mathbb{O}_k$ if and only if $f_{k_1,k_2}(S) \in \mathbb{O}_k$.

Thus, we have $\forall [M_1]_\sim, [M_2]_\sim \in \mathscr{M}/_\sim$

$$\begin{aligned}
[M_1]_\sim \boxplus [M_2]_\sim = [M_1 \oplus M_2]_\sim &= \left\{ P^\mathsf{T} \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} S \,:\, P, S \in \mathbb{O} \right\} \\
&= \left\{ (f_{m_1,m_2}(P))^\mathsf{T} \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} f_{k_1,k_2}(S) \,:\, P, S \in \mathbb{O} \right\} \\
= \Bigg\{ \left(\begin{bmatrix} 0 & I_{m_2} \\ I_{m_1} & 0 \end{bmatrix} P \right)^\mathsf{T} &\begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} \left(\begin{bmatrix} 0 & I_{k_2} \\ I_{k_1} & 0 \end{bmatrix} S \right) \,:\, P, S \in \mathbb{O} \Bigg\} \\
= \left\{ P^\mathsf{T} \left(\begin{bmatrix} 0 & I_{m_1} \\ I_{m_2} & 0 \end{bmatrix} \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} \begin{bmatrix} 0 & I_{k_2} \\ I_{k_1} & 0 \end{bmatrix} \right) S \,:\, P, S \in \mathbb{O} \right\} \\
= \left\{ P^\mathsf{T} \begin{bmatrix} M_2 & 0 \\ 0 & M_1 \end{bmatrix} S \,:\, P, S \in \mathbb{O} \right\} &= [M_2 \oplus M_1]_\sim = [M_2]_\sim \boxplus [M_1]_\sim.
\end{aligned}$$

Consequently, $\mathscr{M}/_\sim$ together with $\boxplus$ form an algebraic structure specified in the following proposition that we have just proved:

Proposition 2. *Let $\mathscr{M}/_\sim$ be the quotient set (3.20) of $\mathscr{M}$ and let $\boxplus : (\mathscr{M}/_\sim)^2 \longrightarrow \mathscr{M}/_\sim$ be the direct summation defined on $\mathscr{M}/_\sim$ by (3.21). Then the ordered pair*

$$(\mathscr{M}/_\sim, \boxplus)$$

forms the structure of commutative monoid.

3.4.1 Remarks on connection of both monoids & notation

The (commutative) monoid $(\mathscr{M}/_\sim, \boxplus)$ from Proposition 2 can be seen as the quotient monoid of the (non-commutative) monoid $(\mathscr{M}, \oplus)$ from Proposition 1 modulo the orthogonal equivalence $\sim$, i.e., symbolically

$$\boxplus \;=\; \oplus/_\sim\,, \qquad (\mathscr{M}/_\sim, \boxplus) = (\mathscr{M}, \oplus)/_\sim\,. \tag{3.22}$$

Further, since the structure is associative and commutative, we can simply write

$$[M]_\sim = \boxplus_{\ell=1}^{n} [M_\ell]_\sim$$

in order to sum up several summands $[M_j]_\sim \in \mathscr{M}/_\sim$. Finally, we use

$$[M]_\sim \boxdot n = \underbrace{[M]_\sim \boxplus [M]_\sim \boxplus \cdots \boxplus [M]_\sim}_{n \text{ times}};$$

analogous notation $M \odot n$ can be used also for $M \oplus M \oplus \cdots \oplus M$.

3.4.2 Note on further relation between $\oplus$ and $\boxplus$

Recall that the binary operation $\oplus$ can be applied on any two (nonempty) subsets of $\mathscr{M}$. The equivalence classes (3.18) are (nonempty) sets, therefore it can also be applied on them. Since this action is defined entry-wisely, we get the following relations. Let

$$[M_j]_\sim = \{P_j^\mathsf{T} M_j S_j \ : \ P_j, S_j \in \mathbb{O}\}, \ j = 1, 2,$$

then

$$[M_1]_\sim \oplus [M_2]_\sim = \left\{ \begin{bmatrix} P_1^\mathsf{T} M_1 S_1 & 0 \\ 0 & P_2^\mathsf{T} M_2 S_2 \end{bmatrix} \ : \ P_j, S_j \in \mathbb{O}, \ j = 1, 2 \right\}, \qquad (3.23)$$

but

$$[M_1 \oplus M_2]_\sim = \left\{ P^\mathsf{T} \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} S \ : \ P, S \in \mathbb{O} \right\}. \qquad (3.24)$$

We see that generally

$$[M_1]_\sim \oplus [M_2]_\sim \subseteq [M_1]_\sim \boxplus [M_2]_\sim$$

and one could ask whether these two sets are the same.

Lemma 1. *Let* $M_j \in \mathbb{R}^{m_j \times k_j} \subset \mathscr{M}$, $j = 1, 2$. *Then*

$$[M_1]_\sim \oplus [M_2]_\sim = [M_1]_\sim \boxplus [M_2]_\sim$$

if and only if at least one of the following three assertions is true

(i) $m_1 = k_1 = 0$, *i.e.,* $M_1 = 0_{0,0} \in \mathbb{R}^{0 \times 0}$;

(ii) $m_2 = k_2 = 0$, *i.e.,* $M_2 = 0_{0,0} \in \mathbb{R}^{0 \times 0}$;

(iii) $M_1 = 0_{m_1,k_1}$ *and* $M_2 = 0_{m_2,k_2}$.

Note that the items in previous lemma are not disjoint. For example the case $M_1 = M_2 = 0_{0,0}$ belongs to all of them.

Proof. The proof is in *one direction* trivial: If $M_1 = 0_{0,0}$, then $[M_1]_\sim = \{0_{0,0}\}$, $M_1 \oplus M_2 = M_2$, and thus also $[M_1]_\sim \oplus [M_2]_\sim = [M_2]_\sim$; on the other hand $[M_1]_\sim \boxplus [M_2]_\sim = [M_1 \oplus M_2]_\sim = [M_2]_\sim$. Similarly it works if $M_2 = 0_{0,0}$. Finally, if both matrices are zeros, then $M_1 \oplus M_2 = 0_{m,k}$, $m = m_1 + m_2$, $k = k_1 + k_2$, is also a zero matrix, and the class $[0_{m,k}]_\sim$ contains the only matrix for any m and k; see Section 3.3.2.

The *other direction* is a bit more complicated: Recall $M_j \in \mathbb{R}^{m_j \times k_j}$, $j = 1, 2$, and note that the entries of the first set (3.23) have the form

$$(P_1 \oplus P_2)^\mathsf{T}(M_1 \oplus M_2)(S_1 \oplus S_2)$$

while entries of the other set (3.24) have the form

$$P^\mathsf{T}(M_1 \oplus M_2)S.$$

We use *three different ways* of argumentation to prove the other implication for (in general 16) different nonzero patterns of the vector of dimensions $[m_1, k_1, m_2, k_2] \in \mathbb{N}_0^4$. For this purpose we denote by

0	the zero entry,
$\heartsuit$	the entry that may be zero as well as nonzero, and
$\clubsuit$	the nonzero entry.

The *first way* to reach equality of both sets is to guarantee that

$$\begin{aligned} & \forall P \in \mathbb{O}_m, \quad \exists P_j \in \mathbb{O}_{m_j},\ j = 1, 2, \quad P = P_1 \oplus P_2, \\ \text{and at the same time} \quad & \forall S \in \mathbb{O}_k, \quad \exists S_j \in \mathbb{O}_{k_j},\ j = 1, 2, \quad S = S_1 \oplus S_2. \end{aligned}$$

This happens only if $m_1 = 0$ or $m_2 = 0$, and at the same time $k_1 = 0$ or $k_2 = 0$, yielding four possible combinations:

- $m_1 = k_1 = 0$, i.e., $M_1 = 0_{0,0}$ covering patterns $[0, 0, \heartsuit, \heartsuit]$ and case (i);
- $m_2 = k_2 = 0$, i.e., $M_2 = 0_{0,0}$ covering patterns $[\heartsuit, \heartsuit, 0, 0]$ and case (ii);
- $m_1 = k_2 = 0$, i.e., $M_1 = 0_{0,k_1}$ and $M_2 = 0_{m_2,0}$ covering patterns $[0, \heartsuit, \heartsuit, 0]$;
- $m_2 = k_1 = 0$, i.e., $M_1 = 0_{m_1,0}$ and $M_2 = 0_{0,k_2}$ covering patterns $[\heartsuit, 0, 0, \heartsuit]$.

Thus, now we have actually covered in total 9 out of 16 patterns. The first two combinations cover cases (i) and (ii) of the lemma, respectively, and the latter two belong to the case (iii).

The *second way* to reach equality of both sets is to guarantee that both sets have only one element — the empty matrix. This means that $(M_1 \oplus M_2) \in \mathbb{R}^{m \times k}$ has either no rows (i.e., $m = 0$) or no columns (i.e., $k = 0$). Since $m = m_1 + m_2$ and $k = k_1 + k_2$, this happen only if $m_1 = m_2 = 0$ or $k_1 = k_2 = 0$. In other words:

- $m_1 = m_2 = 0$, i.e., $M_1 = 0_{0,k_1}$ and $M_2 = 0_{0,k_2}$ covering patterns $[0, \heartsuit, 0, \heartsuit]$;

- $k_1 = k_2 = 0$, i.e., $M_1 = 0_{m_1,0}$ and $M_2 = 0_{m_2,0}$ covering patterns $[\heartsuit, 0, \heartsuit, 0]$.

The second way covers 7 patterns but only 2 are new; so we have covered in total 11 out of 16 patterns now. Since here we play only with empty, i.e., zero matrices, all these patterns belong to the case (iii) of the lemma.

For the *third way* it is important, that we have already exhausted all the patterns where two or more entries of $[m_1, k_1, m_2, k_2]$ are zeros. Thus, only

$$[\heartsuit, \clubsuit, \clubsuit, \clubsuit], \ [\clubsuit, \heartsuit, \clubsuit, \clubsuit], \ [\clubsuit, \clubsuit, \heartsuit, \clubsuit], \ [\clubsuit, \clubsuit, \clubsuit, \heartsuit], \quad \text{where} \quad \clubsuit > 0,$$

remain to explore (representing actually five remaining patterns). Thus, it is safe to consider $m = m_1 + m_2 > 0$ and $k = k_1 + k_2 > 0$. Hence, in (see (3.24))

$$P^{\mathsf{T}} \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} S = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{matrix} \}m_1 \\ \}m_2 \end{matrix}$$
$$\underbrace{\phantom{X_{11}}}_{k_1} \underbrace{\phantom{X_{12}}}_{k_2}$$

at least one of the blocks X_{12} and X_{21} is nonempty (has at least one row and at least one column). Recall that orthogonal matrices P and S can represent permutation of rows and columns. If at least one of the matrices M_1 and M_2 contains at least one nonzero entry, there always exist such permutation matrices P and S that (one of) the nonempty blocks X_{12} and X_{21} contain that nonzero entry. Since the off-diagonal blocks are always zero in (3.23), we conclude that neither M_1 nor M_2 can contain nonzero entries. Thus, both M_j has to be zero matrices, which belong in the case (iii) of the lemma. ☐

3.5 PARTIAL ORDERING OF BOTH SETS --- POSETS $(\mathscr{M}, \preceq)$ AND $(\mathscr{M}/_\sim, \sqsubseteq)$

The size of matrices, or classes of matrices — more precisely, the dimension of linear vector space whereto they belong is nondecreasing along with direct summation. Even more, if we omit the neutral element $0_{0,0}$ or $[0_{0,0}]_\sim$, the dimension is strictly increasing. This allows us to define a very natural *partial ordering* on $\mathscr{M}$:

$$L \preceq M \qquad \Longleftrightarrow \qquad \exists Y, Z \in \mathscr{M}, \quad M = Y \oplus L \oplus Z, \tag{3.25}$$

and similarly

- $L \prec M$ iff $L \preceq M$ & $L \neq M$ (i.e., $Y \neq 0_{0,0}$ or $Z \neq 0_{0,0}$);
- $L \succeq M$ iff $M \preceq L$;
- $L \succ M$ iff $M \prec L$;

etc. Since the other binary operation $\boxplus$ is commutative, the definition of ordering on $\mathscr{M}/_\sim$ is even simpler:

$$[L]_\sim \sqsubseteq [M]_\sim \qquad \Longleftrightarrow \qquad \exists [Z]_\sim \in \mathscr{M}/_\sim, \quad [M]_\sim = [L]_\sim \boxplus [Z]_\sim, \tag{3.26}$$

and similarly

- $[L]_\sim \sqsubset [M]_\sim$ iff $[L]_\sim \sqsubseteq [M]_\sim$ & $[L]_\sim \neq [M]_\sim$ (i.e., $[Z]_\sim \neq [0_{0,0}]_\sim$);
- $[L]_\sim \sqsupseteq [M]_\sim$ iff $[M]_\sim \sqsubseteq [L]_\sim$;
- $[L]_\sim \sqsupset [M]_\sim$ iff $[M]_\sim \sqsubset [L]_\sim$;

etc. Both relations are clearly linked together

$$L \preceq M \qquad \Longrightarrow \qquad [L]_\sim \sqsubseteq [M]_\sim,$$

the converse of this implication is not true, in general.

It is easy to verify that both relation '$\preceq$' and '$\sqsubseteq$' really form the partial ordering. In particular $\preceq$ satisfies the following properties:

$\forall K, L, M \in \mathscr{M}$,

$$\begin{aligned} \text{(reflexivity)} \quad & M \preceq M, \\ \text{(weak antisymmetry)} \quad & L \preceq M \;\&\; M \preceq L \implies L = M, \\ \text{(transitivity)} \quad & K \preceq L \;\&\; L \preceq M \implies K \preceq M; \end{aligned}$$

and similarly $\sqsubseteq$ satisfies the following properties:

$\forall [K]_\sim, [L]_\sim, [M]_\sim \in \mathscr{M}/_\sim$,

$$\begin{aligned} \text{(reflexivity)} \quad & [M]_\sim \sqsubseteq [M]_\sim, \\ \text{(weak antisymmetry)} \quad & [L]_\sim \sqsubseteq [M]_\sim \;\&\; [M]_\sim \sqsubseteq [L]_\sim \implies [L]_\sim = [M]_\sim, \\ \text{(transitivity)} \quad & [K]_\sim \sqsubseteq [L]_\sim \;\&\; [L]_\sim \sqsubseteq [M]_\sim \implies [K]_\sim \sqsubseteq [M]_\sim. \end{aligned}$$

Consequently, $\mathscr{M}$ and $\mathscr{M}/_\sim$ together with $\preceq$ and $\sqsubseteq$ form structures specified in the following proposition that we have just proved:

Proposition 3. *Let $\mathscr{M}$ be the set of all matrices over the real numbers (3.6), let $\mathscr{M}/_\sim$ be the quotient set (3.20) of $\mathscr{M}$, modulo the orthogonal equivalence $\sim$ (3.17), and let $\preceq$ and $\sqsubseteq$ be binary relations defined on $\mathscr{M}$ and $\mathscr{M}/_\sim$ by (3.25) and (3.26), respectively. Then the ordered pairs*

$$(\mathscr{M}, \preceq) \qquad \text{and} \qquad (\mathscr{M}/_\sim, \sqsubseteq)$$

form partially ordered sets (posets for short).

3.5.1 Remark on connection of both posets

The poset $(\mathscr{M}/_\sim, \sqsubseteq)$ from Proposition 3 can be seen as the quotient poset of the poset $(\mathscr{M}, \preceq)$ from Proposition 3 modulo the orthogonal equivalence $\sim$, i.e., symbolically

$$\sqsubseteq = \preceq /_\sim\,, \qquad (\mathscr{M}/_\sim, \sqsubseteq) = (\mathscr{M}, \preceq)/_\sim\,. \tag{3.27}$$

Compare with Section 3.4.1.

3.5.2 Who precedes whom?

The first relation $L \preceq M$ simply says that the matrix L forms a block on the block-diagonal of the block-diagonal matrix M, nothing more, nothing less.

The second relation $\sqsubseteq$ says essentially the same, but *up to an orthogonal transformation*. To be more specific, let us consider

$$\begin{aligned} L &\in \mathbb{R}^{n\times t}, & s &\equiv \mathrm{rank}(L) \le \min(n,t),\\ M &\in \mathbb{R}^{m\times k}, & r &\equiv \mathrm{rank}(M) \le \min(m,k). \end{aligned}$$

Employing the SVDs of L and M (see also Remark 1) we get: $[L]_\sim \sqsubseteq [M]_\sim$ if and only if

(i) The set of s nonzero singular values of L (including the multiplicities) form a subset of the set of r nonzero singular values of M (including the multiplicities).

(ii) Dimensions of *null-spaces* of L, M, L^T, and M^T satisfy

$$\begin{aligned} \dim(\mathcal{N}(L)) \equiv t - s &\le k - r \equiv \dim(\mathcal{N}(M)),\\ \dim(\mathcal{N}(L^\mathsf{T})) \equiv n - s &\le m - r \equiv \dim(\mathcal{N}(M^\mathsf{T})). \end{aligned}$$

3.6 MATRIX AND QUOTIENT POMONOIDS --- AN ANALOGY TO $(\mathbb{N},\cdot,|)$

Now we are ready to put all the previous observations (see Propositions 1, 2, and 3) together. We formulate the following proposition:

Proposition 4. *Let $\mathscr{M}$ be the set of all matrices over the real numbers (3.6), $\oplus$ the binary operation (3.9), and $\preceq$ the binary relation (3.25) defined on $\mathscr{M}$. Let $\mathscr{M}/_\sim$ be the quotient set (3.20) of $\mathscr{M}$, $\boxplus$ the binary operation (3.21), and $\sqsubseteq$ the binary relation (3.26) defined on $\mathscr{M}/_\sim$. Then the ordered triplets*

$$(\mathscr{M},\oplus,\preceq) \qquad \textit{and} \qquad (\mathscr{M}/_\sim,\boxplus,\sqsubseteq)$$

form the structures of non-commutative and commutative, respectively, partially ordered monoid (pomonoids for short).

3.6.1 Remarks on connection of both pomonoids & naturals

The (commutative) pomonoid $(\mathscr{M}/_\sim,\boxplus,\sqsubseteq)$ from Proposition 4 can be seen as the quotient pomonoid of the (non-commutative) pomonoid $(\mathscr{M},\oplus,\preceq)$ from Proposition 4 modulo the orthogonal equivalence $\sim$, i.e., symbolically

$$(\mathscr{M}/_\sim,\boxplus,\sqsubseteq) = (\mathscr{M},\oplus,\preceq)/_\sim\,. \tag{3.28}$$

Compare with Sections 3.4.1 and 3.5.1.

The structure of pomonoids is particular interesting, especially in the second case, where the binary operation is commutative. An analogous structure can be found, e.g., in positive integers (natural numbers), where the pomonoid $(\mathbb{N}, \cdot, |)$ consists of the set of naturals $\mathbb{N}$, their standard multiplication $\cdot$, and the *'to be a divisor'* relation $|$.

It is easy to see that the similar role as the *number one* in $(\mathbb{N}, \cdot, |)$, is here played by the *neutral entries* of monoids, i.e.,

$$\forall M \in \mathscr{M}, \quad 0_{0,0} \preceq M, \qquad \forall [M]_\sim \in \mathscr{M}/_\sim, \quad [0_{0,0}]_\sim \sqsubseteq [M]_\sim.$$

Much more interesting question can be (see also Section 4.3):

Which entries play the role of primes?

3.6.2 What are the irreducible entries?

The *'prime-like'* entries are usually called irreducible in different kinds of analogies of prime factorizations. The *'prime-like factorization'* itself is then called the irreducible representation.

It is easy to see that the irreducible representation of $M \in \mathbb{R}^{m\times k}$ in $\mathscr{M}$ (in fact in $(\mathscr{M}, \oplus, \preceq)$) means to find the maximal number of matrices $M_\ell \in \mathbb{R}^{m_\ell \times k_\ell}$, $\ell = 1, 2, \ldots, n$ with dimensions as small as possible, such that

$$M = \text{diag}(M_1, M_2, \ldots, M_n) = M_1 \oplus M_2 \oplus \cdots \oplus M_n.$$

The *descriptive* characterization of irreducible objects w.r.t. $\preceq$ seems to be superfluously technical in general. Attempts of such characterization usually end up with programmers-like approaches, or with laconic *constructive* assertion: The irreducible object is a matrix, that is not a direct sum of other two matrices distinct from $0_{0,0}$. On the other hand, decomposing the matrix itself is not so important for us.

Much more important is the irreducible representation w.r.t. $\sqsubseteq$. It is in fact done by the SVD; see Remark 1. Clearly for $M \in \mathbb{R}^{m\times k}$, we get

$$[M]_\sim = \left(\mathop{\boxplus}_{\ell=1}^{\text{min}(m,k)} [\sigma_\ell(M)]_\sim \right) \boxplus \begin{cases} [0_{1,0}]_\sim \boxdot (m-k) & \text{if } m > k \\ [0_{0,0}]_\sim & \text{if } m = k \\ [0_{0,1}]_\sim \boxdot (k-m) & \text{if } m < k \end{cases}. \tag{3.29}$$

Note that in case $m = k$ it is even not necessary to apply $[0_{0,0}]_\sim$ as it is trivial (similarly as the multiplication by 1 in $\mathbb{N}$). In the other two cases, decomposing the empty matrices

$$[0_{t,0}]_\sim = [0_{1,0}]_\sim \boxdot t, \qquad [0_{0,n}]_\sim = [0_{0,1}]_\sim \boxdot n,$$

brings nothing especially interesting, thus might not be necessarily done.

4 EXTENSION TO TUPLES OF MATRICES & MATRICIZATIONS OF TUPLES

It seems that in the previous chapter we have just reinvented the notation for the SVD, but in much worse and less transparent way. And that is exactly what we did. But the reason, why we did it in so detailed way, is that our goal is to generalize these concepts, the terminology, and notation to tuples of matrices.

Let us consider the Cartesian product of a bunch of copies of the set $\mathscr{M}$, i.e., the *Cartesian* (or *outer*) *power*

$$\mathscr{M}^{\zeta} = \{(M_1, M_2, \dots, M_{\zeta}) \ : \ M_j \in \mathbb{R}^{m_j \times k_j}, \ j = 1, 2, \dots, \zeta\}. \tag{4.1}$$

Entries of such set are ordered ζ-tuples of matrices, $\zeta \in \mathbb{N}$. These can be naturally seen as vectors of length ζ over $\mathscr{M}$, or, if $\zeta = \mu\kappa$, $\mu, \kappa \in \mathbb{N}$, as μ-by-κ matrices over $\mathscr{M}$. From this point of view $\mathscr{M}^{\zeta}$, $\mathscr{M}^{\mu\times\kappa} \subset \mathscr{M}(\mathscr{M}) \equiv \mathscr{M}(\mathscr{M}(\mathbb{R}))$.

4.1 TUPLES AS OUTER POWERS OF SIMPLER POMONOIDS

Now we can extend the binary operation $\oplus$, the partial ordering $\preceq$, and the orthogonal equivalence relation $\sim$ to $\mathscr{M}^{\zeta}$, and also the other binary operation $\boxplus$ and partial ordering $\sqsubseteq$ to the other Cartesian product $(\mathscr{M}/_{\sim})^{\zeta}$.

4.1.1 The outer power of $(\mathscr{M}, \oplus, \preceq)$

Let first

$$\oplus^{\zeta} \ : \ (\mathscr{M}^{\zeta})^2 \longrightarrow \mathscr{M}^{\zeta} \qquad \text{and} \qquad \preceq^{\zeta} \ \text{on} \ \mathscr{M}^{\zeta}$$

be a binary operation and a binary relation defined such that

$$(L_1, \dots, L_{\zeta}) \oplus^{\zeta} (M_1, \dots, M_{\zeta}) = (L_1 \oplus M_1, \dots, L_{\zeta} \oplus M_{\zeta})$$

and

$$\begin{aligned} & (L_1, \ldots, L_\zeta) \preceq^\zeta (M_1, \ldots, M_\zeta) \\ \iff & \exists Y_j,\, Z_j \in \mathscr{M}, \quad M_j = Y_j \oplus L_j \oplus Z_j, \quad j = 1, \ldots, \zeta, \\ \iff & \exists (Y_1, \ldots, Y_\zeta),\, (Z_1, \ldots, Z_\zeta) \in \mathscr{M}^\zeta, \\ & (M_1, \ldots, M_\zeta) = (Y_1, \ldots, Y_\zeta) \oplus^\zeta (L_1, \ldots, L_\zeta) \oplus^\zeta (Z_1, \ldots, Z_\zeta), \end{aligned}$$

respectively. It is easy to see that all the required properties (the associativity of $\oplus^\zeta$, the existence of neutral entry $(0_{0,0}, \ldots, 0_{0,0})$ w.r.t. $\oplus^\zeta$; and also the reflexivity, weak antisymmetry, and transitivity of $\preceq^\zeta$) are satisfied. Thus, we get the following proposition:

Proposition 5. *Let $\mathscr{M}^\zeta$ be the Cartesian power defined in (4.1), $\oplus^\zeta$, the binary operation, and $\preceq^\zeta$ the binary relation defined on $\mathscr{M}^\zeta$ as above. Then the ordered triplet*

$$(\mathscr{M}^\zeta, \oplus^\zeta, \preceq^\zeta)$$

forms the structure of non-commutative pomonoid.

4.1.2 The outer power of $(\mathscr{M}/_\sim, \boxplus, \sqsubseteq)$

Similarly we can define a relation $\sim^\zeta$ on $\mathscr{M}^\zeta$ as follows

$$(L_1, \ldots, L_\zeta) \sim^\zeta (M_1, \ldots, M_\zeta) \qquad \iff \qquad L_j \sim M_j, \quad j = 1, \ldots, \zeta$$

and show that this relation is reflexive, symmetric, and transitive, and thus it is an equivalence — also called the *orthogonal equivalence*. Then we can define the equivalence classes and the quotient set (the set of the classes),

$$\Big[(M_1, \ldots, M_\zeta)\Big]_{\sim^\zeta} \qquad \text{and} \qquad \mathscr{M}^\zeta/_{\sim^\zeta}\,,$$

respectively. Clearly

$$\Big[(M_1, \ldots, M_\zeta)\Big]_{\sim^\zeta} = \Big([M_1]_\sim, \ldots, [M_\zeta]_\sim\Big) \qquad \text{and thus} \qquad \mathscr{M}^\zeta/_{\sim^\zeta} = (\mathscr{M}/_\sim)^\zeta.$$

Further, we extend the binary operation $\boxplus$ and the binary relation $\sqsubseteq$ componentwisely to

$$\boxplus^\zeta \;:\; ((\mathscr{M}/_\sim)^\zeta)^2 \longrightarrow (\mathscr{M}/_\sim)^\zeta \qquad \text{and} \qquad \sqsubseteq^\zeta \;\text{ on } (\mathscr{M}/_\sim)^\zeta$$

similarly as in Section 4.1.1. Finally, we get the following proposition:

Proposition 6. *Let $(\mathscr{M}/_\sim)^\zeta$ be quotient set of $\mathscr{M}^\zeta$ (4.1), $\boxplus^\zeta$ the binary operation, and $\sqsubseteq^\zeta$ the binary relation defined on $(\mathscr{M}/_\sim)^\zeta$ as above. Then the ordered triplet*

$$((\mathscr{M}/_\sim)^\zeta, \boxplus^\zeta, \sqsubseteq^\zeta)$$

forms the structure of commutative pomonoid.

4.1.3 Remarks on connections among all pomonoids

Since the (non-commutative) pomonoid $(\mathscr{M}^\zeta, \oplus^\zeta, \preceq^\zeta)$ from Proposition 5 is the natural Cartesian power of the (non-commutative) pomonoid $(\mathscr{M}, \oplus, \preceq)$ from Proposition 4, we can write symbolically

$$(\mathscr{M}^\zeta, \oplus^\zeta, \preceq^\zeta) = (\mathscr{M}, \oplus, \preceq)^\zeta\,; \tag{4.2}$$

see Section 4.1.1.

Similarly the (commutative) pomonoid $((\mathscr{M}/_\sim)^\zeta, \boxplus^\zeta, \sqsubseteq^\zeta)$ from Proposition 6 is the natural Cartesian power of the (commutative) pomonoid $(\mathscr{M}/_\sim, \boxplus, \sqsubseteq)$ from Proposition 4, we can write symbolically

$$((\mathscr{M}/_\sim)^\zeta, \boxplus^\zeta, \sqsubseteq^\zeta) = (\mathscr{M}/_\sim, \boxplus, \sqsubseteq)^\zeta\,; \tag{4.3}$$

see Section 4.1.2. Using the already introduced notation (3.28), we obtain

$$((\mathscr{M}/_\sim)^\zeta, \boxplus^\zeta, \sqsubseteq^\zeta) = ((\mathscr{M}, \oplus, \preceq)/_\sim)^\zeta\,; \tag{4.4}$$

see Section 3.6.1.

Finally, note that the (non-commutative) pomonoid $((\mathscr{M}/_\sim)^\zeta, \boxplus^\zeta, \sqsubseteq^\zeta)$ from Section 4.1.2 can be seen as the quotient pomonoid of the (commutative) pomonoid $(\mathscr{M}^\zeta, \oplus^\zeta, \preceq^\zeta)$ from Section 4.1.1 modulo the orthogonal equivalence $\sim$, i.e., symbolically

$$\boxplus^\zeta = \oplus^\zeta/_\sim\,, \qquad \sqsubseteq^\zeta = \preceq^\zeta/_\sim\,, \qquad ((\mathscr{M}/_\sim)^\zeta, \boxplus^\zeta, \sqsubseteq^\zeta) = (\mathscr{M}^\zeta, \oplus^\zeta, \preceq^\zeta)/_\sim\,. \tag{4.5}$$

Compare with Sections 3.4.1, 3.5.1, and 3.6.1.

Consequently, putting (4.4), (4.5) and (4.2) together yields

$$((\mathscr{M}, \oplus, \preceq)/_\sim)^\zeta = ((\mathscr{M}/_\sim)^\zeta, \boxplus^\zeta, \sqsubseteq^\zeta) = (\mathscr{M}^\zeta, \oplus^\zeta, \preceq^\zeta)/_\sim = ((\mathscr{M}, \oplus, \preceq)^\zeta)/_\sim\,, \tag{4.6}$$

i.e., a sort of commutativity relation between the quotient (modulo the orthogonal equivalence) reduction and the Cartesian power.

4.2 ALIGNMENTS, MATRICIZATIONS, & TRANSFORMATIONS OF TUPLES

As one can see, the straightforward extension to tuples of matrices brings nothing especially new. All the things (derivations and definitions) are done component-wisely, independently for each member of the tuple.

Therefore, we first restrict the variability of tuples by some additional conditions — the tuple alignment, i.e., we focus on some subsets of (4.1). Then we introduce the tuple matricization. Finally, we also restrict the variability of allowed orthogonal transformations.

4.2.1 Tuple alignment

To simplify the exposition, we explain these concepts on a particular example (to do it in full generality is out of the scope of this text). Consider, e.g.,

$$\mathscr{M}^4 = \big\{ (M_1, M_2, M_3, M_4) \ : \ M_j \in \mathbb{R}^{m_j \times k_j} \subset \mathscr{M} \big\}\,. \tag{4.7}$$

By tuple alignment (TA) we understand any given set of conditions on dimensions m_j and k_j of the tuple, e.g.,

$$\mathsf{TA} = \big\{\, m_1 - m_2 = 0\,,\ \ m_1 + m_3 - m_4 = 0\,,\ \ k_1 + k_2 - k_3 = 0 \,\big\}. \tag{4.8}$$

These conditions clearly relate the individual members of the tuple — in our example we see that (among others) the first two matrices M_1 and M_2 must have the same number of rows. The set of all tuples satisfying all these conditions is denoted

$$\mathscr{M}^4_{\mathsf{TA}} \subseteq \mathscr{M}^4. \tag{4.9}$$

4.2.2 Tuple matricization

By matricization of a tuple we understand any given mapping from the set of tuples of matrices (or its subset) back to the set of matrices. This allows us to deal with tuples as with standard matrices. The alignment of the tuple, moreover, allows us to concatenate individual members of the tuple in specific ways. Following our example (4.7)–(4.9) we can consider

$$\mathsf{TM} \ : \ \mathscr{M}^4_{\mathsf{TA}} \ \longrightarrow \ \mathscr{M} \tag{4.10}$$

that acts, e.g.,

$$\mathsf{TM}\Big((M_1, M_2, M_3, M_4) \Big) = \left[\begin{array}{c|c} \begin{array}{c|c} M_2 & M_1 \\ \hline \multicolumn{2}{c}{M_3} \end{array} & M_4 \end{array} \right] = M \in \mathbb{R}^{m \times k}, \tag{4.11}$$

where $m = m_1 + m_3 = m_2 + m_3 = m_4$, $k = k_1 + k_2 + k_4 = k_3 + k_4$.

It is easy to see that the quadruple (M_1, M_2, M_3, M_4) can also be considered as the *partitioning* of M. Moreover (since $\mathscr{M}$ contains also empty matrices), any matrix M can be partitioned in this way. For our purpose it is, however, more suitable to choose the way of alignment and matricization, not the way of partitioning.

Note that the matricization (or partitioning) in this example is '*incompatible*'. For our purpose (the core problem analysis) we need to work only with '*compatible*' matricizations — the individual blocks appear in regular rectangular '*matrix-like*' grid, e.g.:

$$\begin{bmatrix} M_1 & M_2 \\ M_3 & M_4 \end{bmatrix}, \quad \begin{bmatrix} M_1 \\ M_2 \\ M_3 \end{bmatrix}, \quad \begin{bmatrix} M_2 & M_1 \end{bmatrix}, \quad \text{but also} \quad \begin{bmatrix} M_3 & M_1 \\ M_2^{\mathsf{T}} & 0 \end{bmatrix},$$

etc. Furthermore, note that without any alignment conditions, i.e., with

$$\mathsf{TA} = \emptyset, \qquad \text{we get} \qquad \mathscr{M}^{\zeta}_{\mathsf{TA}} = \mathscr{M}^{\zeta}_{\emptyset} = \mathscr{M}^{\zeta}.$$

One of possible matricizations can be then realized by the direct summation

$$\mathsf{TM}\Big((M_1, \dots, M_\zeta)\Big) = M_1 \oplus \dots \oplus M_\zeta = \begin{bmatrix} M_1 & & \\ & \ddots & \\ & & M_\zeta \end{bmatrix},$$

we call it trivial matricization.

4.2.3 Tuple transformation

By tuple transformation induced by the already given alignment TA and matricization TM we understand binary relation $\sim_{\mathsf{TT}}$ on $\mathscr{M}^{\zeta}_{\mathsf{TA}}$ defined for

$$\mathfrak{L} = (L_1, \dots, L_\zeta),\ \mathfrak{M} = (M_1, \dots, M_\zeta)\ \in \mathscr{M}^{\zeta}_{\mathsf{TA}}$$

such that

$$\mathfrak{L} \sim_{\mathsf{TT}} \mathfrak{M} \qquad \Longleftrightarrow \qquad \Big(\ \mathfrak{L} \sim^{\zeta} \mathfrak{M} \quad \wedge \quad \mathsf{TM}(\mathfrak{L}) \sim \mathsf{TM}(\mathfrak{M})\ \Big). \tag{4.12}$$

This relation is an algebraic equivalence on $\mathscr{M}^{\zeta}_{\mathsf{TA}}$.

Let us clarify this on our example (4.7)–(4.11): Recall that

$$\mathfrak{L} \sim^{4} \mathfrak{M} \quad \Longleftrightarrow \quad \mathfrak{L} = g(\mathfrak{M}) = \Big(P_1^{\mathsf{T}} M_1 S_1,\ P_2^{\mathsf{T}} M_2 S_2,\ P_3^{\mathsf{T}} M_3 S_3,\ P_4^{\mathsf{T}} M_4 S_4\Big),$$

where

$$P_j \in \mathbb{O}_{m_j}, \quad S_j \in \mathbb{O}_{k_j}, \quad j = 1, 2, 3, 4,$$

and mappings g (orthogonal transformations) given by these eight matrices represent elements of the group

$$\mathbb{G} = \Big(\mathbb{O}_{m_1} \times \mathbb{O}_{k_1}\Big) \times \Big(\mathbb{O}_{m_2} \times \mathbb{O}_{k_2}\Big) \times \Big(\mathbb{O}_{m_3} \times \mathbb{O}_{k_3}\Big) \times \Big(\mathbb{O}_{m_4} \times \mathbb{O}_{k_4}\Big).$$

Replacing this group by any of its subgroup $\mathbb{P}$ causes the modification of the equivalence relation (formally from $\sim^4$ to, let say $\sim_{\mathbb{P}}$), but it stays an algebraic equivalence, since the subgroup is still a group; see the proof in Section 3.3). (Note that in general this replacement also causes increasing number of classes, and decreasing number of elements within a class.)

The other part of the definition of the newly introduced relation (4.12) says

$$\mathsf{TM}(\mathfrak{L}) = \mathsf{TM}(g(\mathfrak{M})) \sim \mathsf{TM}(\mathfrak{M}),$$

i.e., the matricizations of the original and transformed tuple are orthogonally equivalent. The matricization, therefore, dictates the structure of the new equivalence

$$\begin{aligned}\left[\begin{array}{c|c}\begin{array}{c|c} L_2 & L_1 \\ \hline \multicolumn{2}{c}{L_3}\end{array} & L_4\end{array}\right] &= \left[\begin{array}{c|c}\begin{array}{c|c} P_1^{\mathsf{T}}M_2S_2 & P_1^{\mathsf{T}}M_1S_1 \\ \hline \multicolumn{2}{c}{P_3^{\mathsf{T}}M_3(S_2\oplus S_1)}\end{array} & (P_1\oplus P_3)^{\mathsf{T}}M_4S_4\end{array}\right] \\ &= \begin{bmatrix} P_1^{\mathsf{T}} & 0 \\ 0 & P_3^{\mathsf{T}}\end{bmatrix}\left[\begin{array}{c|c}\begin{array}{c|c} M_2 & M_1 \\ \hline \multicolumn{2}{c}{M_3}\end{array} & M_4\end{array}\right]\begin{bmatrix} S_2 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_4\end{bmatrix}.\end{aligned} \tag{4.13}$$

We immediately see that some of the orthogonal groups $\mathbb{O}_{\dots}$ must be replaced in the product $\mathbb{G}$ by their proper subgroups:

$$\begin{aligned} m_1+m_3=m_4 \ &\in \mathsf{TA} &\quad\Longrightarrow\quad& \mathbb{O}_{m_4} \text{ is replaced by } \mathbb{O}_{m_1}\times\mathbb{O}_{m_3}, \\ k_1+k_2=k_3 \ &\in \mathsf{TA} &\quad\Longrightarrow\quad& \mathbb{O}_{k_3} \text{ is replaced by } \mathbb{O}_{k_1}\times\mathbb{O}_{k_2}. \end{aligned}$$

Moreover, some of the orthogonal groups $\mathbb{O}_{\dots}$ that appear more than once in $\mathbb{G}$ represent in fact the same instance of the group, i.e., the corresponding orthogonal matrices appear in more than one products:

$$\begin{aligned} m_1=m_2 \ &\in \mathsf{TA} &\quad\Longrightarrow\quad& P_2 \text{ is replaced by } P_1, \\ m_1+m_3=m_4 \ &\in \mathsf{TA} &\quad\Longrightarrow\quad& P_4 \text{ is replaced by } P_1\oplus P_3, \\ k_1+k_2=k_3 \ &\in \mathsf{TA} &\quad\Longrightarrow\quad& S_3 \text{ is replaced by } S_1\oplus S_2. \end{aligned}$$

Any of these replacements reduce $\mathbb{G}$ to some of its proper subgroup. We denote the remaining subgroup symbolically

$$\mathsf{TT}=\mathsf{TT}(\mathsf{TA},\mathsf{TM}); \tag{4.14}$$

in our example, this subgroup is isomorphic to

$$\mathbb{P}=\Big(\mathbb{O}_{m_1}\times\mathbb{O}_{m_3}\Big)\times\Big(\mathbb{O}_{k_1}\times\mathbb{O}_{k_2}\times\mathbb{O}_{k_4}\Big).$$

Since (4.14) is the subgroup of $\mathbb{G}$, the binary relation $\sim_{\mathsf{TT}}$ represents an algebraic equivalence on $\mathscr{M}^{\zeta}_{\mathsf{TA}}$.

4.3 CLASSES AND POMONOIDS OF ALIGNED TUPLES

At the end of this chapter, we just briefly mention how the general concepts work in the context of aligned tuples — we will follow our example (4.7)–(4.14). For $\mathfrak{L}$ and $\mathfrak{M}\in\mathscr{M}^4_{\mathsf{TA}}$:

- The equivalence class has the form

$$\begin{aligned}[\mathfrak{M}]_{\sim_{\mathsf{TT}}} = \Big\{\Big(&P_1^{\mathsf{T}}M_1S_1, P_1^{\mathsf{T}}M_2S_2,\ P_3^{\mathsf{T}}M_3(S_2\oplus S_1),\ (P_1\oplus P_3)^{\mathsf{T}}M_4S_4\Big)\ : \\ &P_1\in\mathbb{O}_{m_1},\ P_3\in\mathbb{O}_{m_3},\ S_1\in\mathbb{O}_{k_1},\ S_2\in\mathbb{O}_{k_2},\ S_4\in\mathbb{O}_{k_4}\Big\}.\end{aligned}$$

- The direct sum of two aligned tuples results again in an aligned tuple

$$\mathsf{TM}(\mathfrak{L} \oplus^4 \mathfrak{M}) = \left[\begin{array}{c|c} \begin{array}{c|c} L_2 \oplus M_2 & L_1 \oplus M_1 \\ \hline \multicolumn{2}{c}{L_3 \oplus M_3} \end{array} & L_4 \oplus M_4 \end{array}\right].$$

  Clearly if, e.g., L_1 and L_2 have the same number of rows, M_1 and M_2 have the same number of rows, then also $L_1 \oplus M_1$ and $L_2 \oplus M_2$ have the same number of rows, etc.
- The ordering works fully the same as for general tuples; using the previous item, we see that, e.g., $\mathfrak{M} \preceq^4 (\mathfrak{L} \oplus^4 \mathfrak{M})$ and $\mathfrak{L} \preceq^4 (\mathfrak{L} \oplus^4 \mathfrak{M})$.

Now we are able to build up pomonoids

$$(\mathscr{M}^{\zeta}_{\mathsf{TA}}, \oplus^{\zeta}, \preceq^{\zeta}) \qquad \text{and} \qquad (\mathscr{M}^{\zeta}_{\mathsf{TA}}/_{\sim_{\mathsf{TT}}}, \boxplus^{\zeta}, \sqsubseteq^{\zeta}).$$

The second one can again be seen as the quotient pomonoid of the first one, modulo the modified orthogonal equivalence $\sim_{\mathsf{TT}}$.

The key question is:

Which entries are irreducible (prime-like) entries in these pomonoids?

especially in the second one. This question is very general, seems to be very difficult to answer, and definitely is out of the scope of this text. In the next chapter we focus on the simplest case of aligned tuples — the row-aligned pairs of aligned matrices.

5 CLOSER LOOK AT ROW-ALIGNED PAIRS OF MATRICES

From this moment on, we focus on the simplest nontrivial case of aligned tuple — the aligned *pair*. Since this work is motivated by linear approximation problems $AX \approx B$ (1.6), we slightly modify our notation: instead of M_1 and M_2 we will use A and B, respectively, in particular

$$\mathscr{M}^2 = \big\{(A, B) \ : \ A \in \mathbb{R}^{m_A \times n},\ B \in \mathbb{R}^{m_B \times d}\big\}\,.$$

Both matrices must have (in accordance to our problem, and without loss of generality) the same number of rows $m = m_A = m_B$, i.e.,

$$\mathsf{TA} = \{m_A - m_B = 0\}\,. \tag{5.1}$$

The matricization then simply concatenates both matrices — we choose (again in accordance to our convenience, and without loss of generality) the '*reverse*' order

$$\mathsf{TM}\Big((A, B)\Big) = \left[\begin{array}{cc} B & A \end{array}\right] \in \mathbb{R}^{m \times k}, \quad k = d + n. \tag{5.2}$$

The tuple transformations (actually pair transformations) induced by this alignment and matricization take the form

$$\mathsf{TT} \ : \quad \left[\begin{array}{cc} B & A \end{array}\right] \sim P^{\mathsf{T}} \left[\begin{array}{cc} B & A \end{array}\right] \left[\begin{array}{cc} R & 0 \\ 0 & Q \end{array}\right] = \left[\begin{array}{cc} P^{\mathsf{T}}BR & P^{\mathsf{T}}AQ \end{array}\right], \tag{5.3}$$

where $(P, Q, R) \in \mathbb{O}_m \times \mathbb{O}_n \times \mathbb{O}_d$; recall Section 1.2.

5.1 $\mathbb{GP}$: THE SET OF ALL GENERAL PROBLEMS

We are studying general linear approximation problems of the form $AX \approx B$ and we are solving them by orthogonally invariant minimization (the TLS method in particular). This means that we are interested exactly in the aligned ordered pairs up to the orthogonal transformation. Thus, the set of such problems fits exactly to the set

$$\mathbb{GP} \equiv \mathscr{M}^2_{\mathsf{TA}}/_{\sim_{\mathsf{TT}}}\,, \tag{5.4}$$

where TA is given by (5.1) and TT by (5.3)

5.1.1 Simplification of notation for general problems

Because the length of tuple, its alignment, matricization, and thus also transformations are fixed since this moment, we simplify the notation a bit in order to make the text more transparent. In particular we will :

- refer to the classes of orthogonally equivalent pairs directly by their representatives,
- omit the superscript ^{2} in direct summation or ordering signs, and
- omit the subscript $_{\mathsf{TT}}$ in equivalence sign,

i.e., for example

$$\Big[(A_\alpha, B_\alpha)\Big]_{\sim_{\mathsf{TT}}} \sqsubseteq^2 \Big[(A, B)\Big]_{\sim_{\mathsf{TT}}} = \Big[(A_\alpha, B_\alpha)\Big]_{\sim_{\mathsf{TT}}} \boxplus^2 \Big[(A_\beta, B_\beta)\Big]_{\sim_{\mathsf{TT}}}$$

will be simply written as

$$(A_\alpha, B_\alpha) \sqsubseteq (A, B) \sim (A_\alpha, B_\alpha) \boxplus (A_\beta, B_\beta).$$

5.1.2 Composition of general problems

The most important manipulation with problems for us is the composition of problems realized by the direct summation

$$\boxplus \;:\; \mathbb{GP}^2 \longrightarrow \mathbb{GP}. \tag{5.5}$$

Note that we will also use this binary operation sign in a less rigorous way. Let

$$A_j X_j \approx B_j, \qquad A_j \in \mathbb{R}^{m_j \times n_j}, \quad X_j \in \mathbb{R}^{n_j \times d_j}, \quad B_j \in \mathbb{R}^{m_j \times d_j},$$

be two linear approximation problems, i.e., $(A_j, B_j) \in \mathbb{GP}$, $j = \alpha, \beta$. Except for the standard usage

$$(A_\alpha, B_\alpha) \boxplus (A_\beta, B_\beta) = \left(\begin{bmatrix} A_\alpha & 0 \\ 0 & A_\beta \end{bmatrix}, \begin{bmatrix} B_\alpha & 0 \\ 0 & B_\beta \end{bmatrix} \right), \tag{5.6}$$

we also use it directly for matricizations (which is a bit conflicting with some of the previous notation, but — as we believe — understandable), i.e.,

$$\begin{bmatrix} B_\alpha & A_\alpha \end{bmatrix} \boxplus \begin{bmatrix} B_\beta & A_\beta \end{bmatrix} = \left[\begin{array}{cc|cc} B_\alpha & 0 & A_\alpha & 0 \\ 0 & B_\beta & 0 & A_\beta \end{array} \right]. \tag{5.7}$$

Occasionally we use it also for the whole approximation problems

$$\left\{A_\alpha X_\alpha \approx B_\alpha\right\} \boxplus \left\{A_\beta X_\beta \approx B_\beta\right\} = \left\{\left[\begin{array}{cc} A_\alpha & 0 \\ 0 & A_\beta \end{array}\right] X \approx \left[\begin{array}{cc} B_\alpha & 0 \\ 0 & B_\beta \end{array}\right]\right\}. \tag{5.8}$$

Note that X does not have to be equal to the direct sum of X_α and X_β in general; see [4, Section 5.2, Example 5.4]

5.1.3 Note on composition of degenerated problems

Recall that the set of all matrices contain also empty matrices (i.e., with zero number of rows or columns). Problem that consists of at least one empty matrix is called degenerated. Now we briefly look what happens when we are composing problems that may be degenerated. Two most interesting cases are:

- If $n_\beta = 0$, i.e., $A_\beta = 0_{m_j,0}$, then

$$\left[\begin{array}{cc} B_\alpha & A_\alpha \end{array}\right] \boxplus \left[\begin{array}{cc} B_\beta & A_\beta \end{array}\right] = \left[\begin{array}{cc|c} B_\alpha & 0 & A_\alpha \\ 0 & B_\beta & 0 \end{array}\right] \in \mathbb{R}^{(m_\alpha+m_\beta)\times((d_\alpha+d_\beta)+n_\alpha)}.$$

- If $d_\beta = 0$, i.e., $B_\beta = 0_{m_j,0}$, then

$$\left[\begin{array}{cc} B_\alpha & A_\alpha \end{array}\right] \boxplus \left[\begin{array}{cc} B_\beta & A_\beta \end{array}\right] = \left[\begin{array}{c|cc} B_\alpha & A_\alpha & 0 \\ 0 & 0 & A_\beta \end{array}\right] \in \mathbb{R}^{(m_\alpha+m_\beta)\times(d_\alpha+(n_\alpha+n_\beta))}.$$

The full list of compositions regarding degenerated problems can be found in Table 5.1 (page 67).

5.2 $\mathbb{CP}$: THE SET OF ALL CORE PROBLEMS

By core problem we understand any linear approximation problem $AX \approx B$ i.e., $(A, B) \in \mathbb{GP}$ satisfying conditions

$*$(CP1) The matrix A is of *full column rank*.

$*$(CP2) The matrix $B \in \mathbb{R}^{\overline{m}\times\overline{d}}$ is of *full column rank*.

$*$(CP3) Matrices $U_i^\mathsf{T} B$ are of *full row rank*, where columns of U_i represent basis of: either the left singular subspace of A corresponding to the ith largest singular value, for $i = 1, \ldots, \xi$; or the space $\mathcal{N}(A^\mathsf{T})$, for $i = \xi + 1$.

We denote the set of all core problems $\mathbb{CP}$. Clearly

$$\mathbb{CP} \subsetneq \mathbb{GP} \tag{5.9}$$

is a proper subset of the set of all general problems; i.e., there are linear approximation problems that are not core problems.

Note that from (CP1)–(CP3) other properties of core problems can be derived, particularly useful will be:

(CP4) The matrix $[B, A]$ is of *full row rank*.

(CP6) Multiplicities of singular values of the matrix A are bounded by rank(B).

See [6], [7], or [11, Appendix A].

5.2.1 Core problem reduction

The core problem theory (see in particular [22], [6]) says, that for each linear approximation problem

$$AX \approx B, \qquad A \in \mathbb{R}^{m\times n}, \quad X \in \mathbb{R}^{n\times d}, \quad B \in \mathbb{R}^{m\times d},$$

there always exist orthogonal matrices $P \in \mathbb{O}_m$, $Q \in \mathbb{O}_n$, and $R \in \mathbb{O}_d$, such that

$$P^{\mathsf{T}} \left[\begin{array}{cc} B & A \end{array}\right] \left[\begin{array}{cc} R & 0 \\ 0 & Q \end{array}\right] = \left[\begin{array}{cc|cc} B_1 & 0 & A_{11} & 0 \\ 0 & 0 & 0 & A_{22} \end{array}\right], \tag{5.10}$$

i.e.,

$$\left[\begin{array}{cc} A_{11} & 0 \\ 0 & A_{22} \end{array}\right] \left[\begin{array}{cc} X_{11} & X_{12} \\ X_{21} & X_{22} \end{array}\right] \approx \left[\begin{array}{cc} B_1 & 0 \\ 0 & 0 \end{array}\right]$$

i.e.,

$$A_{11}X_{11} \approx B_1, \quad A_{11}X_{12} \approx 0, \quad A_{22}X_{21} \approx 0, \quad A_{22}X_{22} \approx 0,$$

where

$$A_{11}X_{11} \approx B_1, \qquad A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}, \quad X_{11} \in \mathbb{R}^{\overline{n}\times\overline{d}}, \quad B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}},$$

is the core problem. Thus, for any $(A, B) \in \mathbb{GP}$

$$\left[\begin{array}{cc} B & A \end{array}\right] \sim \left[\begin{array}{cc|cc} B_1 & 0 & A_{11} & 0 \\ 0 & 0 & 0 & A_{22} \end{array}\right].$$

We use the notation suitable for matrix right-hand side case (see [6]) here, but the vector right-hand side case $Ax \approx b$ (see [22]) represents only a special case with $X = [x] \in \mathbb{R}^{n\times 1}$, $B = [b] \in \mathbb{R}^{m\times 1}$,

$$\left[\begin{array}{cc} B & A \end{array}\right] = \left[\begin{array}{cc} b & A \end{array}\right] \sim \left[\begin{array}{c|cc} b_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{array}\right] = \left[\begin{array}{cc|cc} B_1 & 0_{\overline{m},0} & A_{11} & 0 \\ 0 & 0_{m-\overline{m},0} & 0 & A_{22} \end{array}\right],$$

and $B_1 = [b_1] \in \mathbb{R}^{\overline{m}\times 1}$. The core problem is given uniquely up to an orthogonal transformation, i.e., up to the equivalence $\sim$, i.e.,

$$\forall\,(A, B) \in \mathbb{GP} \;:\; \quad \exists!\,(A_{11}, B_1) \in \mathbb{CP};$$

see again [22], [6]. We call this mapping the core problem reduction

$$\text{CPR} \;:\; \mathbb{GP} \longrightarrow \mathbb{CP}, \tag{5.11}$$

and symbolically write as

$$\text{CPR}\Big(\left[\begin{array}{cc} B & A \end{array}\right]\Big) = \left[\begin{array}{cc} B_1 & A_{11} \end{array}\right] \qquad \text{or} \qquad \left[\begin{array}{cc} B & A \end{array}\right] \xrightarrow{\text{CPR}} \left[\begin{array}{cc} B_1 & A_{11} \end{array}\right].$$

5.2.2 Note on degenerated core problems

Since $\mathbb{GP}$ contains also the degenerated problems, it is necessary to look how the core problem reduction performs on them. In most cases of degenerated problems, one or a combination of conditions (CP1), (CP2), and (CP4) (on full column or row ranks of matrices A_{11}, B_1, and $[B_1, A_{11}]$), and once also (CP6) (on multiplicities of singular values of A_{11}) imply that CPR results in the fully degenerated (i.e., with no rows and no columns in the system matrix as well as in the right-hand side) core problem

$$\left[\ B_1 \mid A_{11}\ \right] = \left[\ 0_{0,0} \mid 0_{0,0}\ \right] \in \mathbb{CP}.$$

The list of all degenerated problems and results of CPRs (including the key properties (CPℓ) that clarifies the result) can be found in Table 5.2 (page 67).

However, there is one degenerated problem that is not reduced to the fully degenerated one by the CPR, in general. Let

$$A \in \mathbb{R}^{m\times 0}, \qquad B \in \mathbb{R}^{m\times d}, \qquad r = \mathsf{rank}(B).$$

Consider SVDs of both matrices, the first one is rather formal

$$A = U_A \Sigma_A V_A^{\mathsf{T}}, \quad U_A = I_m \in \mathbb{O}_m, \quad \Sigma_A = 0_{m,0} \in \mathbb{R}^{m\times 0}, \quad V_A = 0_{0,0} \in \mathbb{O}_0,$$

the other is

$$B = U_B \Sigma_B V_B^{\mathsf{T}}, \quad U_B \in \mathbb{O}_m, \quad \Sigma_B = \begin{bmatrix} B_1 & 0_{r,d-r} \\ 0_{m-r,r} & 0_{m-r,d-r} \end{bmatrix} \in \mathbb{R}^{m\times d}, \quad V_B \in \mathbb{O}_d,$$

and the diagonal matrix with (nonzero) singular values

$$B_1 \in \mathbb{R}^{r\times r} \qquad \text{is square invertible.}$$

Then for $P = U_B$, $Q = V_A = 0_{0,0}$, and $R = V_B$ we get

$$\begin{aligned}\left[\ B \mid A\ \right] \sim P^{\mathsf{T}} \left[\ B \mid A\ \right] \begin{bmatrix} R & 0 \\ 0 & Q \end{bmatrix} &= U_B^{\mathsf{T}} \left[\ B \mid 0_{m,0}\ \right] \begin{bmatrix} V_B & 0 \\ 0 & 0_{0,0} \end{bmatrix} = \left[\ \Sigma_B \mid 0_{m,0}\ \right] \\ &= \left[\begin{array}{cc|c} B_1 & 0_{r,d-r} & 0_{r,0} \\ 0_{m-r,r} & 0_{m-r,d-r} & 0_{m-r,0} \end{array}\right] = \left[\begin{array}{cc|cc} B_1 & 0_{r,d-r} & A_{11} & 0_{r,0} \\ 0_{m-r,r} & 0_{m-r,d-r} & 0_{m-r,0} & A_{22} \end{array}\right],\end{aligned}$$

where $A_{11} = 0_{r,0} \in \mathbb{R}^{r\times 0}$ and $A_{22} = 0_{m-r,0} \in \mathbb{R}^{(m-r)\times 0}$.

Obviously, this transformation (according to the structure of the result) formally resembles the core problem revealing transformation. It remains to verify, whether $[B_1, A_{11}]$ satisfies the properties (CP1)–(CP3):

- Matrix A_{11} is the empty (zero) matrix, it has $\mathsf{rank}(A_{11}) = 0$ and zero columns, i.e., it is of *full column rank*: (CP1) holds.
- Matrix B_1 is square invertible, i.e., it is of *full column rank*: (CP2) holds.

- The SVD of $A_{11} = I_r \, 0_{r,0} \, 0_{0,0}^{\mathsf{T}}$ is analogous to the SVD of A; A_{11} has no singular values, the whole $\mathbb{R}^r$ is the null-space of A_{11}^{T} and columns of $U_1 = I_r$ represents its basis. Since B_1 is invertible, then $U_1^{\mathsf{T}} B_1 = I_r B_1 = B_1$ is of *full row rank*: (CP3) holds.

Consequently, any square invertible matrix B_1 of order r together with empty matrix $A_{11} = 0_{r,0}$ represent a core problem. Since square invertible matrix is characterized by nonzero determinant, we may define the whole set

$$\Big\{(A_{11}, B_1) \in \mathbb{GP} \;\;:\;\; A_{11} = 0_{r,0},\; B_1 \in \mathbb{R}^{r\times r},\; \text{det}(B_1) \neq 0,\; r \in \mathbb{N}_0\Big\} \subsetneq \mathbb{CP} \qquad (5.12)$$

of degenerated core problems. Since $\text{det}(0_{0,0}) = 1$, the set contains also the fully degenerated core problem for $r = 0$. Note that nontrivial degenerated core problems are also observed in paper [4, Theorem 3.2].

5.2.3 Composition and core problem reduction — they properties and interplay

Now we have two important tools to work with approximation problems: the composition $\boxplus$ (5.5) and the core problem reduction CPR (5.11). It would be useful to look on its interplay.

First of all, the composition is defined on the set of all problems $\mathbb{GP}$, but it can be applied also on its proper subset of core problems $\mathbb{CP}$. It has been shown (see [4, Theorems 3.1 and 3.2]) that

$$\boxplus \;:\; \mathbb{CP}^2 \longrightarrow \mathbb{CP}. \qquad (5.13)$$

In other words the set of core problems is closed w.r.t. the composition. More specifically

$$(A_{11,\alpha}, B_{1,\alpha}),\; (A_{11,\beta}, B_{1,\beta}) \;\in \mathbb{CP} \quad\Longleftrightarrow\quad (A_{11,\alpha}, B_{1,\alpha}) \boxplus (A_{11,\beta}, B_{1,\beta}) \;\in \mathbb{CP};$$

naturally, including the degenerated core problems.

Secondly, the core problem reduction is also defined on the whole set of all problems $\mathbb{GP}$ and can be restricted to the proper subset of core problems $\mathbb{CP}$. From the properties of core problems and the construction of the reduction (see [22], [6]), however, follows that the core problem reduction of a problem which already is a core problem is trivial. In other words

$$\text{CPR} \;:\; \mathbb{CP} \longrightarrow \mathbb{CP}, \qquad (5.14)$$

is the identity mapping

$$\forall\,(A_{11}, B_1) \in \mathbb{CP} \;:\quad \text{CPR}\Big((A_{11}, B_1)\Big) = (A_{11}, B_1). \qquad (5.15)$$

From this point of view:

The core problem reduction is an orthogonal projection from $\mathbb{GP}$ onto $\mathbb{CP}$

Table 5.1: All possible shapes of $[B_\alpha, A_\alpha] \boxplus [B_\beta, A_\beta]$ according to different dimensions of A_j, B_j, $j = \alpha, \beta$, being (non)zero.

<table>
<tr><th>zero dims.</th><th>no</th><th>$m_\alpha = 0$</th><th>$m_\beta = 0$</th><th>$m_\alpha = m_\beta = 0$</th></tr>
<tr><td>no</td><td>$\left[\begin{array}{cc|cc} B_\alpha & 0 & A_\alpha & 0 \\ 0 & B_\beta & 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{cc|cc} 0 & B_\beta & 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{cc|cc} B_\alpha & 0 & A_\alpha & 0 \end{array}\right]$</td><td>$\left[\begin{array}{cc|cc} 0_{0,d_\alpha} & 0_{0,d_\beta} & 0_{0,n_\alpha} & 0_{0,n_\beta} \end{array}\right]$</td></tr>
<tr><td>$n_\alpha = 0$</td><td>$\left[\begin{array}{cc|c} B_\alpha & 0 & 0 \\ 0 & B_\beta & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{cc|c} 0 & B_\beta & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{cc|c} B_\alpha & 0 & 0 \end{array}\right]$</td><td>$\left[\begin{array}{cc|c} 0_{0,d_\alpha} & 0_{0,d_\beta} & 0_{0,n_\beta} \end{array}\right]$</td></tr>
<tr><td>$n_\beta = 0$</td><td>$\left[\begin{array}{cc|c} B_\alpha & 0 & A_\alpha \\ 0 & B_\beta & 0 \end{array}\right]$</td><td>$\left[\begin{array}{cc|c} 0 & B_\beta & 0 \end{array}\right]$</td><td>$\left[\begin{array}{cc|c} B_\alpha & 0 & A_\alpha \end{array}\right]$</td><td>$\left[\begin{array}{cc|c} 0_{0,d_\alpha} & 0_{0,d_\beta} & 0_{0,n_\alpha} \end{array}\right]$</td></tr>
<tr><td>$d_\alpha = 0$</td><td>$\left[\begin{array}{c|cc} 0 & A_\alpha & 0 \\ B_\beta & 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|cc} B_\beta & 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|cc} 0 & A_\alpha & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|cc} 0_{0,d_\beta} & 0_{0,n_\alpha} & 0_{0,n_\beta} \end{array}\right]$</td></tr>
<tr><td>$d_\beta = 0$</td><td>$\left[\begin{array}{c|cc} B_\alpha & A_\alpha & 0 \\ 0 & 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|cc} 0 & 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|cc} B_\alpha & A_\alpha & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|cc} 0_{0,d_\alpha} & 0_{0,n_\alpha} & 0_{0,n_\beta} \end{array}\right]$</td></tr>
<tr><td>$n_\alpha = n_\beta = 0$</td><td>$\begin{bmatrix} B_\alpha & 0 \\ 0 & B_\beta \end{bmatrix}$</td><td>$\begin{bmatrix} 0 & B_\beta \end{bmatrix}$</td><td>$\begin{bmatrix} B_\alpha & 0 \end{bmatrix}$</td><td>$\begin{bmatrix} 0_{0,d_\alpha} & 0_{0,d_\beta} \end{bmatrix}$</td></tr>
<tr><td>$d_\alpha = d_\beta = 0$</td><td>$\begin{bmatrix} A_\alpha & 0 \\ 0 & A_\beta \end{bmatrix}$</td><td>$\begin{bmatrix} 0 & A_\beta \end{bmatrix}$</td><td>$\begin{bmatrix} A_\alpha & 0 \end{bmatrix}$</td><td>$\begin{bmatrix} 0_{0,n_\alpha} & 0_{0,n_\beta} \end{bmatrix}$</td></tr>
<tr><td>$n_\alpha = d_\alpha = 0$</td><td>$\left[\begin{array}{c|c} 0 & 0 \\ B_\beta & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|c} B_\beta & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0 & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,d_\beta} & 0_{0,n_\beta} \end{array}\right]$</td></tr>
<tr><td>$n_\beta = d_\beta = 0$</td><td>$\left[\begin{array}{c|c} B_\alpha & A_\alpha \\ 0 & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0 & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|c} B_\alpha & A_\alpha \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,d_\alpha} & 0_{0,n_\alpha} \end{array}\right]$</td></tr>
<tr><td>$n_\alpha = d_\beta = 0$</td><td>$\left[\begin{array}{c|c} B_\alpha & 0 \\ 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0 & A_\beta \end{array}\right]$</td><td>$\left[\begin{array}{c|c} B_\alpha & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,d_\alpha} & 0_{0,n_\beta} \end{array}\right]$</td></tr>
<tr><td>$n_\beta = d_\alpha = 0$</td><td>$\left[\begin{array}{c|c} 0 & A_\alpha \\ B_\beta & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|c} B_\beta & 0 \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0 & A_\alpha \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,d_\beta} & 0_{0,n_\alpha} \end{array}\right]$</td></tr>
<tr><td>$n_\alpha = n_\beta$
$= d_\alpha = 0$</td><td>$\begin{bmatrix} 0 \\ B_\beta \end{bmatrix}$</td><td>$B_\beta$</td><td>$0_{m_\alpha,d_\beta}$</td><td>$0_{0,d_\beta}$</td></tr>
<tr><td>$n_\alpha = n_\beta$
$= d_\beta = 0$</td><td>$\begin{bmatrix} B_\alpha \\ 0 \end{bmatrix}$</td><td>$0_{m_\beta,d_\alpha}$</td><td>$B_\alpha$</td><td>$0_{0,d_\alpha}$</td></tr>
<tr><td>$n_\alpha = d_\alpha$
$= d_\beta = 0$</td><td>$\begin{bmatrix} 0 \\ A_\beta \end{bmatrix}$</td><td>$A_\beta$</td><td>$0_{m_\alpha,n_\beta}$</td><td>$0_{0,n_\beta}$</td></tr>
<tr><td>$n_\beta = d_\alpha$
$= d_\beta = 0$</td><td>$\begin{bmatrix} A_\alpha \\ 0 \end{bmatrix}$</td><td>$0_{m_\beta,n_\alpha}$</td><td>$A_\alpha$</td><td>$0_{0,n_\alpha}$</td></tr>
<tr><td>$n_\alpha = n_\beta = d_\alpha$
$= d_\beta = 0$</td><td>$\begin{bmatrix} 0_{m_\alpha,0} \\ 0_{m_\beta,0} \end{bmatrix}$</td><td>$0_{m_\beta,0}$</td><td>$0_{m_\alpha,0}$</td><td>$0_{0,0}$</td></tr>
</table>

Table 5.2: All possible shapes of $[B, A]$ and CPR($[B, A]$) $= [B_1, A_{11}]$ according to different dimensions of A and B being (non)zero. Below most of the reductions we mention the key property (CPℓ) to get the result.

<table>
<tr><th>zero dims.</th><th>no</th><th>$m = 0$</th></tr>
<tr><td>no</td><td>$\left[\begin{array}{c|c} B & A \end{array}\right] \xrightarrow{\text{CPR}} \left[\begin{array}{c|c} B_1 & A_{11} \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,d} & 0_{0,n} \end{array}\right] \xrightarrow[\text{(CP1 \& 2)}]{\text{CPR}} \left[\begin{array}{c|c} 0_{0,0} & 0_{0,0} \end{array}\right]$</td></tr>
<tr><td>$n = 0$</td><td>$\left[\begin{array}{c|c} B & 0_{m,0} \end{array}\right] \xrightarrow{\text{CPR}} \left[\begin{array}{c|c} B_1 & 0_{\overline{m},0} \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,d} & 0_{0,0} \end{array}\right] \xrightarrow[\text{(CP2)}]{\text{CPR}} \left[\begin{array}{c|c} 0_{0,0} & 0_{0,0} \end{array}\right]$</td></tr>
<tr><td>$d = 0$</td><td>$\left[\begin{array}{c|c} 0_{m,0} & A \end{array}\right] \xrightarrow[\text{(CP6)}]{\text{CPR}} \left[\begin{array}{c|c} 0_{0,0} & 0_{0,0} \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,0} & 0_{0,n} \end{array}\right] \xrightarrow[\text{(CP1)}]{\text{CPR}} \left[\begin{array}{c|c} 0_{0,0} & 0_{0,0} \end{array}\right]$</td></tr>
<tr><td>$n = d = 0$</td><td>$\left[\begin{array}{c|c} 0_{m,0} & 0_{m,0} \end{array}\right] \xrightarrow[\text{(CP4)}]{\text{CPR}} \left[\begin{array}{c|c} 0_{0,0} & 0_{0,0} \end{array}\right]$</td><td>$\left[\begin{array}{c|c} 0_{0,0} & 0_{0,0} \end{array}\right] \xrightarrow[\text{trivial}]{\text{CPR}} \left[\begin{array}{c|c} 0_{0,0} & 0_{0,0} \end{array}\right]$</td></tr>
</table>

A real interplay of both tools can be obtained, when we start combining them, i.e., when we consider a core problem reduction of a problem composition. We formulate it via a commutative diagram in the following theorem.

Theorem 1. *Let* (A_α, B_α) *and* (A_β, B_β) *be two general problems from* $\mathbb{GP}$. *Then*

$$\begin{tikzcd}
(A_\alpha, B_\alpha) \arrow[r, "\text{CPR}"] \arrow[d] & (A_{11,\alpha}, B_{1,\alpha}) \arrow[d] \\
(A_\alpha, B_\alpha) \boxplus (A_\beta, B_\beta) \arrow[r, "\text{CPR}"] & (A_{11,\alpha}, B_{1,\alpha}) \boxplus (A_{11,\beta}, B_{1,\beta}) \\
(A_\beta, B_\beta) \arrow[r, "\text{CPR}"] \arrow[u] & (A_{11,\beta}, B_{1,\beta}) \arrow[u]
\end{tikzcd} \tag{5.16}$$

i.e., composition of two problems and core problem reductions commute.

Note that the assertion of the previous theorem can also be rewritten as

$$\text{CPR}\Big(\begin{bmatrix} B_\alpha & A_\alpha \end{bmatrix} \boxplus \begin{bmatrix} B_\beta & A_\beta \end{bmatrix}\Big) = \text{CPR}\Big(\begin{bmatrix} B_\alpha & A_\alpha \end{bmatrix}\Big) \boxplus \text{CPR}\Big(\begin{bmatrix} B_\beta & A_\beta \end{bmatrix}\Big).$$

Proof. The *outer way* (first reduce, then compose): The core problem reduction of general problems (A_j, B_j) results in $(A_{11,j}, B_{1,j})$ satisfying (CP1)–(CP3), $j = \alpha, \beta$, i.e., there exist orthogonal matrices P_j, Q_j, and R_j such that

$$\begin{bmatrix} B_j & A_j \end{bmatrix} \sim P_j^\mathsf{T} \begin{bmatrix} B_j & A_j \end{bmatrix} \begin{bmatrix} R_j & 0 \\ 0 & Q_j \end{bmatrix} = \left[\begin{array}{cc|cc} B_{1,j} & 0 & A_{11,j} & 0 \\ 0 & 0 & 0 & A_{22,j} \end{array}\right].$$

Composition of both core problems then yields

$$\begin{bmatrix} B_{1,\alpha} & A_{11,\alpha} \end{bmatrix} \boxplus \begin{bmatrix} B_{1,\beta} & A_{11,\beta} \end{bmatrix} = \left[\begin{array}{cc|cc} B_{1,\alpha} & 0 & A_{11,\alpha} & 0 \\ 0 & B_{1,\beta} & 0 & A_{11,\beta} \end{array}\right],$$

which is a core problem by (5.14).

The *inner way* (first compose, then reduce): Composition of (A_j, B_j) yields

$$\begin{bmatrix} B_\alpha & A_\alpha \end{bmatrix} \boxplus \begin{bmatrix} B_\beta & A_\beta \end{bmatrix} = \left[\begin{array}{cc|cc} B_\alpha & 0 & A_\alpha & 0 \\ 0 & B_\beta & 0 & A_\beta \end{array}\right]. \tag{5.17}$$

This composition is orthogonally equivalent to

$$\begin{aligned}
&\begin{bmatrix} P_\alpha & 0 \\ 0 & P_\beta \end{bmatrix}^\mathsf{T} \left[\begin{array}{cc|cc} B_\alpha & 0 & A_\alpha & 0 \\ 0 & B_\beta & 0 & A_\beta \end{array}\right] \left[\begin{array}{cc|cc} R_\alpha & 0 & 0 & 0 \\ 0 & R_\beta & 0 & 0 \\ \hline 0 & 0 & Q_\alpha & 0 \\ 0 & 0 & 0 & Q_\beta \end{array}\right] \\
&= \left[\begin{array}{cc|cc} P_\alpha^\mathsf{T} B_\alpha R_\alpha & 0 & P_\alpha^\mathsf{T} A_\alpha Q_\alpha & 0 \\ 0 & P_\beta^\mathsf{T} B_\beta R_\beta & 0 & P_\beta^\mathsf{T} A_\beta Q_\beta \end{array}\right] \\
&= \left[\begin{array}{cc|cc} \begin{bmatrix} B_{1,\alpha} & 0 \\ 0 & 0 \end{bmatrix} & \mathbf{0} & \begin{bmatrix} A_{11,\alpha} & 0 \\ 0 & A_{22,\alpha} \end{bmatrix} & \mathbf{0} \\ \mathbf{0} & \begin{bmatrix} B_{1,\beta} & 0 \\ 0 & 0 \end{bmatrix} & \mathbf{0} & \begin{bmatrix} A_{11,\beta} & 0 \\ 0 & A_{22,\beta} \end{bmatrix} \end{array}\right]
\end{aligned}$$

$$= \left[\begin{array}{cccc|cccc} B_{1,\alpha} & 0 & 0 & 0 & A_{11,\alpha} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{22,\alpha} & 0 & 0 \\ 0 & 0 & B_{1,\beta} & 0 & 0 & 0 & A_{11,\beta} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & A_{22,\beta} \end{array}\right]. \tag{5.18}$$

Consider a permutation matrix of the following form and recall its action

$$\Pi = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix}, \qquad \Pi \begin{bmatrix} \clubsuit \\ \heartsuit \\ \spadesuit \\ \diamondsuit \end{bmatrix} = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} \clubsuit \\ \heartsuit \\ \spadesuit \\ \diamondsuit \end{bmatrix} = \begin{bmatrix} \clubsuit \\ \spadesuit \\ \heartsuit \\ \diamondsuit \end{bmatrix},$$

where identities in Π are of given suitable dimensions. Note that Π and Π^{T} have the same block structure (and thus also same structure of action). Further note that matrix Π is orthogonal so $\Pi\Pi^{\mathsf{T}} = \Pi^{\mathsf{T}}\Pi = I$.

By employing three of such matrices Π_P, Π_Q, and Π_R, we get a problem orthogonally equivalent to (5.18) while permuting rows and columns of (5.18) as follows

$$\begin{aligned} &\sim \Pi_P^{\mathsf{T}} \left[\begin{array}{cccc|cccc} B_{1,\alpha} & 0 & 0 & 0 & A_{11,\alpha} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{22,\alpha} & 0 & 0 \\ 0 & 0 & B_{1,\beta} & 0 & 0 & 0 & A_{11,\beta} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & A_{22,\beta} \end{array}\right] \left[\begin{array}{c|c} \Pi_R & 0 \\ \hline 0 & \Pi_Q \end{array}\right] \\ &= \left[\begin{array}{cccc|cccc} B_{1,\alpha} & 0 & 0 & 0 & A_{11,\alpha} & 0 & 0 & 0 \\ 0 & B_{1,\beta} & 0 & 0 & 0 & A_{11,\beta} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{22,\alpha} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & A_{22,\beta} \end{array}\right] \\ &= \left[\begin{array}{cc|cc} \begin{bmatrix} B_{1,\alpha} & 0 \\ 0 & B_{1,\beta} \end{bmatrix} & 0 & \begin{bmatrix} A_{11,\alpha} & 0 \\ 0 & A_{11,\beta} \end{bmatrix} & 0 \\ 0 & 0 & 0 & \begin{bmatrix} A_{22,\alpha} & 0 \\ 0 & A_{22,\beta} \end{bmatrix} \end{array}\right] \end{aligned} \tag{5.19}$$

Consequently, the composition (5.17) is orthogonally equivalent to the last problem in (5.19), which has the structure of (5.10). Thus,

$$\left[\begin{array}{cc|cc} B_{1,\alpha} & 0 & A_{11,\alpha} & 0 \\ 0 & B_{1,\beta} & 0 & A_{11,\beta} \end{array}\right]$$

could potentially be a core problem if it satisfies (CP1)–(CP3). And we already know it does as it is the same problem that we get by the outer way. $\square$

5.3 DE-COMPOSING (CORE) PROBLEM INTO IRREDUCIBLE REPRESENTATION

Now we are ready to start to talk about our ultimate goal — in fact reversing the process of composing problems, i.e., to decompose the given problem. We want to decompose it as much as possible, i.e., into parts that are no further decomposable, or in other words, that are irreducible, or '*prime-like*' entries in the pomonoid $\mathbb{GP}$.

Note that while composing, dimensions of the resulting problem are sums of respective dimensions of individual subproblems. Thus, having a given problem its dimensions cannot decrease by its composition with another one — but some of them, even all of them may stay the same, if we compose our problem with the fully degenerated one $(0_{0,0}, 0_{0,0})$. This fully degenerated problem w.r.t. composition plays similar role as number one w.r.t. multiplication — it is the neutral entry.

While reversing the composition we, therefore, ignore the (always available) possibility of decomposing given the problem to itself and $(0_{0,0}, 0_{0,0})$ (similarly as we ignore the multiplication by one in the prime decomposition). In other words, we consider only nontrivial decompositions, i.e., on the set

$$\mathbb{GP} \setminus \Big\{(0_{0,0}, 0_{0,0})\Big\}.$$

Let us introduce for $(A, B) \in \mathbb{GP}$, $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times d}$, quantity

$$\mathfrak{D} \; : \; \mathbb{GP} \longrightarrow \mathbb{N}_0, \qquad \mathfrak{D}\Big((A, B)\Big) = m + n + d, \tag{5.20}$$

which moreover satisfies

$$\mathfrak{D}\Big((A, B)\Big) = 0 \qquad \Longleftrightarrow \qquad (A, B) = (0_{0,0}, 0_{0,0}).$$

Thus, $\mathfrak{D}$ is positive on $\mathbb{GP} \setminus \{(0_{0,0}, 0_{0,0})\}$. Consequently, nontrivial decomposition of

$$(A, B) \;\longrightarrow\; (A_\alpha, B_\alpha) \boxplus (A_\beta, B_\beta),$$

where $A_j \in \mathbb{R}^{m_j\times n_j}$, $B_j \in \mathbb{R}^{m_j\times d_j}$, $j = \alpha, \beta$, is always followed by strict decrease of quantity $\mathfrak{D}$, i.e.,

$$\mathfrak{D}\Big((A, B)\Big) > \mathfrak{D}\Big((A_j, B_j)\Big), \qquad j = \alpha, \beta.$$

Therefore, any sequence of decompositions is finite, so it ends with problems that are not further decomposable, i.e., they are our irreducible entries.

5.3.1 Step I: Revealing core problem $[B_1, A_{11}]$ as decomposition

Comparing the result of composition of two problems (5.7),

$$\left[\begin{array}{cc} B_\alpha & A_\alpha \end{array}\right] \boxplus \left[\begin{array}{cc} B_\beta & A_\beta \end{array}\right] = \left[\begin{array}{cc|cc} B_\alpha & 0 & A_\alpha & 0 \\ 0 & \boxed{B_\beta} & 0 & A_\beta \end{array}\right].$$

with the core problem revealing transformation (5.10),

$$\left[\begin{array}{cc} B & A \end{array}\right] \sim P^{\mathsf{T}} \left[\begin{array}{cc} B & A \end{array}\right] \left[\begin{array}{cc} R & 0 \\ 0 & Q \end{array}\right] = \left[\begin{array}{cc|cc} B_1 & 0 & A_{11} & 0 \\ 0 & \boxed{0} & 0 & A_{22} \end{array}\right],$$

we immediately see that revealing the core problem essentially does a decomposition

$$\left[\begin{array}{cc} B & A \end{array}\right] \sim \underbrace{\left[\begin{array}{cc} B_1 & A_{11} \end{array}\right]}_{\mathsf{CPR}\left(\left[\begin{array}{cc} B & A \end{array}\right]\right)} \boxplus \underbrace{\left[\begin{array}{cc} 0_{m-\overline{m},d-\overline{d}} & A_{22} \end{array}\right]}_{\mathsf{CPC}\left(\left[\begin{array}{cc} B & A \end{array}\right]\right)}. \tag{5.21}$$

We call the other problem the core problem complement (CPC for short). Note that in the standard single right-hand side case (i.e., with nonzero b), $d = \overline{d} = 1$ and the complement is degenerated with empty right-hand side.

5.3.2 Step II: Note on decomposition of the core problem complement $[0_{m-\overline{m},d-\overline{d}}, A_{22}]$

The decomposition of the core problem complement (A_{22}, B_2) is rather trivial, because it has zero right-hand side $B_2 = 0_{m-\overline{m},d-\overline{d}}$. Recall that $A_{22} \in \mathbb{R}^{m-\overline{m},n-\overline{n}}$, and denote for simplicity $\mu \equiv m - \overline{m}$, $\nu \equiv n - \overline{n}$, $\delta \equiv d - \overline{d}$.

The complement can always be decomposed into two degenerated problems (see (3.11)),

$$\mathsf{CPC}\left(\left[\begin{array}{cc} B & A \end{array}\right]\right) = \left[\begin{array}{cc} 0_{\mu,\delta} & A_{22} \end{array}\right] \sim \left[\begin{array}{cc} 0_{0,\delta} & 0_{0,0} \end{array}\right] \boxplus \left[\begin{array}{cc} 0_{\mu,0} & A_{22} \end{array}\right]. \tag{5.22}$$

The first one has no rows, the second has empty right-hand side with no columns. (If $d = \overline{d}$, this decomposition is not necessary, because the first problem is fully degenerated.)

The subproblem $[0_{\mu,0}, A_{22}]$ can further be decomposed (see (3.29)) as follows

$$\left[\begin{array}{cc} 0_{\mu,0} & A_{22} \end{array}\right] \sim \left(\mathop{\boxplus}_{\ell=1}^{\mathsf{min}(\mu,\nu)} \left[\begin{array}{cc} 0_{1,0} & \sigma_\ell(A_{22}) \end{array}\right] \right) \boxplus \left\{ \begin{array}{ll} \left[\begin{array}{cc} 0_{\mu-\nu,0} & 0_{\mu-\nu,0} \end{array}\right] & \text{if } \mu > \nu \\ \left[\begin{array}{cc} 0_{0,0} & 0_{0,0} \end{array}\right] & \text{if } \mu = \nu \\ \left[\begin{array}{cc} 0_{0,0} & 0_{0,\nu-\mu} \end{array}\right] & \text{if } \mu < \nu \end{array} \right., \tag{5.23}$$

where $\sigma_\ell(A_{22})$ denotes the ℓth largest singular value of A_{22} including multiplicities and zero singular values. (If $\mu = \nu$, the last problem is again fully degenerated and can be ignored.)

5.3.3 Step III: Extracting degenerated component $[B_{1,\beta}, 0_{\overline{m},0}]$ from the core problem

Recall that the core problem might be composed while some of its components might be degenerated (see(5.12) or [4, Theorem 3.2]), i.e.,

$$\mathsf{CPR}\Big(\left[\begin{array}{cc} B & A \end{array}\right]\Big) = \left[\begin{array}{cc} B_1 & A_{11} \end{array}\right] \sim \left[\begin{array}{cc} B_{1,\alpha} & A_{11,\alpha} \end{array}\right] \boxplus \left[\begin{array}{cc} B_{1,\beta} & 0_{\overline{m}_\beta,0} \end{array}\right]. \tag{5.24}$$

Equivalently, there exist orthogonal matrices P_1, Q_1, R_1, such that

$$\begin{aligned} P_1^\mathsf{T} \left[\begin{array}{cc} B_1 & A_{11} \end{array}\right] \left[\begin{array}{cc} R_1 & 0 \\ 0 & Q_1 \end{array}\right] &= \left[\begin{array}{cc|cc} B_{1,\alpha} & 0 & A_{11,\alpha} & 0_{\overline{m}_\alpha,0} \\ 0 & B_{1,\beta} & 0 & 0_{\overline{m}_\beta,0} \end{array}\right] \\ &= \left[\begin{array}{cc|c} B_{1,\alpha} & 0 & A_{11,\alpha} \\ 0 & B_{1,\beta} & 0 \end{array}\right]. \end{aligned} \tag{5.25}$$

Dimensions of matrices are $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$, $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$, $A_{11,\alpha} \in \mathbb{R}^{\overline{m}_\alpha\times\overline{n}_\alpha}$ ($\overline{n} = \overline{n}_\alpha$), $B_1 \in \mathbb{R}^{\overline{m}_\alpha\times\overline{d}_\alpha}$, and $B_{1,\beta}$ is square invertible matrix of order $\overline{m}_\beta$. (If $\overline{m}_\beta = 0$, then $B_{1,\beta} = 0_{0,0}$ and the β-component is fully degenerated.)

To extract the degenerated subproblem we employ the SVD of $B_1 = U\Sigma V^\mathsf{T}$. It can be written in the form of the direct sum of SVDs of $B_{1,j} = U_j\Sigma_j V_j^\mathsf{T}$, $j = \alpha, \beta$, as follows

$$B_1 = P_1 \left[\begin{array}{cc} B_{1,\alpha} & 0 \\ 0 & B_{1,\beta} \end{array}\right] R_1^\mathsf{T} = \underbrace{\left(P_1 \left[\begin{array}{cc} U_\alpha & 0 \\ 0 & U_\beta \end{array}\right]\right)}_{U} \underbrace{\left[\begin{array}{cc} \Sigma_\alpha & 0 \\ 0 & \Sigma_\beta \end{array}\right]}_{\Sigma} \underbrace{\left(R_1 \left[\begin{array}{cc} U_\alpha & 0 \\ 0 & U_\beta \end{array}\right]\right)^\mathsf{T}}_{V}.$$

From the property (CP2) of core problems we know that Σ, Σ_α, and Σ_β are of full column rank; moreover, since $B_{1,\beta}$ is square invertible, Σ_β is, too. Then

$$U^\mathsf{T} A_{11} = \left(P_1 \left[\begin{array}{cc} U_\alpha & 0 \\ 0 & U_\beta \end{array}\right]\right)^\mathsf{T} \left(P_1 \left[\begin{array}{c} A_{11,\alpha} \\ 0 \end{array}\right] Q_1^\mathsf{T}\right) = \left[\begin{array}{c} U_\alpha^\mathsf{T} A_{11,\alpha} \\ 0 \end{array}\right] Q_1^\mathsf{T}.$$

We see that this matrix contains information only form the α-component; the degenerated subproblem, i.e., the β-component is completely dampen in the result. More precisely, the result still depends on the orthogonal matrix Q_1 (one of the matrices from the block-partitioning revealing transformation (5.25)), however, it only mixes columns of the result together, i.e., the 2-norms of individual rows of the result are independent on Q_1. Consequently,

$$U^\mathsf{T} \left[\begin{array}{cc} B_1 & A_{11} \end{array}\right] \left[\begin{array}{cc} V & 0 \\ 0 & I_{\overline{n}} \end{array}\right] = \left[\begin{array}{cc|c} \Sigma_\alpha & 0 & U_\alpha^\mathsf{T} A_{11,\alpha} Q_1^\mathsf{T} \\ 0 & \Sigma_\beta & 0 \end{array}\right].$$

We see that the singular values of $B_{1,\beta}$, the right-hand side of the degenerated subproblem correspond to the zero rows in matrix $U^\mathsf{T} A_{11}$. But we do not have any a-priori information about which singular value of B_1 belongs to the α- and which to the β-component, i.e., we do not have the SVD in this particular form of the direct sum.

Thus, consider (rather general) SVD of B_1 in the standard form, i.e.,

$$B_1 = U\Sigma V^{\mathsf{T}}, \quad \Sigma = \left[\begin{array}{c} \mathsf{diag}(\sigma_1(B_1), \ldots, \sigma_{\overline{d}}(B_1)) \\ 0_{\overline{m}-\overline{d},\overline{d}} \end{array} \right], \quad \sigma_1(B_1) \geq \cdots \geq \sigma_{\overline{d}}(B_1) > 0;$$

recall that B_1 is of full column rank. Then

$$U^{\mathsf{T}} \left[\begin{array}{cc} B_1 & A_{11} \end{array} \right] \left[\begin{array}{cc} V & 0 \\ 0 & I_{\overline{n}} \end{array} \right] = \left[\begin{array}{c|c} \Sigma & U^{\mathsf{T}} A_{11} \end{array} \right].$$

Let $\ell \in \{1, 2, \ldots, \overline{d}\}$ and let $\sigma_\ell(B_1)$ be such singular value for which

$$e_\ell^{\mathsf{T}}(U^{\mathsf{T}} A_{11}) = u_\ell^{\mathsf{T}} A_{11} = 0_{1,\overline{n}}, \tag{5.26}$$

i.e., the ℓth row of $U^{\mathsf{T}} A_{11}$ is zero; here e_ℓ denotes the ℓth Euclidean vector and $u_\ell = U e_\ell$. Consider the permutation matrix

$$\Pi_{s,\ell} = \left[\begin{array}{ccc} I_{\ell-1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & I_{s-\ell} & 0 \end{array} \right] \in \mathbb{R}^{s \times s}$$

that moves the last entry to the ℓth position when applied from the left on a vector of length s (i.e., $\Pi_{s,\ell}^{\mathsf{T}}$ moves the ℓth entry to the last position). Then

$$\Pi_{\overline{m},\ell}^{\mathsf{T}} \Sigma \Pi_{\overline{d},\ell} = \left[\begin{array}{cc} \boxed{\begin{array}{c} \mathsf{diag}(\sigma_1(B_1), \ldots, \sigma_{\ell-1}(B_1), \sigma_{\ell+1}(B_1), \ldots, \sigma_{\overline{d}}(B_1)) \\ 0_{\overline{m}-\overline{d},\overline{d}-1} \end{array}} & \begin{array}{c} 0_{\overline{d}-1,1} \\ 0_{\overline{m}-\overline{d},1} \end{array} \\ 0_{1,\overline{d}-1} & \boxed{\sigma_\ell(B_1)} \end{array} \right],$$

and clearly

$$\Pi_{\overline{m},\ell}^{\mathsf{T}}(U^{\mathsf{T}} A_{11}) = \left[\begin{array}{c} u_1^{\mathsf{T}} A_{11} \\ \vdots \\ u_{\ell-1}^{\mathsf{T}} A_{11} \\ u_{\ell+1}^{\mathsf{T}} A_{11} \\ \vdots \\ u_{\overline{m}-1}^{\mathsf{T}} A_{11} \\ u_\ell^{\mathsf{T}} A_{11} \end{array} \right] = \left[\begin{array}{c} \boxed{\begin{array}{c} u_1^{\mathsf{T}} A_{11} \\ \vdots \\ u_{\ell-1}^{\mathsf{T}} A_{11} \\ u_{\ell+1}^{\mathsf{T}} A_{11} \\ \vdots \\ u_{\overline{m}-1}^{\mathsf{T}} A_{11} \end{array}} \\ 0_{1,\overline{n}} \end{array} \right].$$

Finally,

$$\left(U\Pi_{\overline{m},\ell} \right)^{\mathsf{T}} \left[\begin{array}{cc} B_1 & A_{11} \end{array} \right] \left[\begin{array}{cc} V\Pi_{\overline{d},\ell} & 0 \\ 0 & I_{\overline{n}} \end{array} \right] = \left[\begin{array}{cc} \Pi_{\overline{m},\ell}^{\mathsf{T}} \Sigma \Pi_{\overline{d},\ell} & \Pi_{\overline{m},\ell}^{\mathsf{T}}(U^{\mathsf{T}} A_{11}) \end{array} \right]$$

has the structure of the form (5.25) (see the boxes above), with orthogonal matrices $P_1 = U\Pi_{\overline{m},\ell}$, $Q_1 = I_{\overline{n}}$, $R_1 = V\Pi_{\overline{d},\ell}$. Clearly, we can do the same job for all ℓ ($1 \leq \ell \leq \overline{d}$), for which (5.26) holds, but this is not enough.

Let the ℓth singular value be of multiplicity t, i.e.,

$$\sigma_{\ell-1}(B_1) > \sigma_\ell(B_1) = \cdots = \sigma_{\ell+t-1}(B_1) > \sigma_{\ell+t}(B_1).$$

Let further

$$\text{rank}\left(\left[\ u_\ell, \ldots, u_{\ell+t-1}\ \right]^\mathsf{T} A_{11}\right) = \tau \le t, \quad \text{where} \quad \left[\ u_\ell, \ldots, u_{\ell+t-1}\ \right]^\mathsf{T} A_{11} \in \mathbb{R}^{t\times\overline{n}}.$$

Then there exist orthogonal matrix $\Psi \in \mathbb{O}(t)$ such that

$$\Psi^\mathsf{T}\left(\left[\ u_\ell, \ldots, u_{\ell+t-1}\ \right]^\mathsf{T} A_{11}\right) = \begin{bmatrix} \clubsuit \\ 0_{t-\tau,\overline{n}} \end{bmatrix}, \quad \text{where} \quad \clubsuit \in \mathbb{R}^{\tau\times\overline{n}} \tag{5.27}$$

is of full row rank. Note that Ψ can be obtained, e.g., by the QR decomposition of $[u_\ell, \ldots, u_{\ell+t-1}]^\mathsf{T} A_{11}$. Consequently

$$\begin{bmatrix} I_{\ell-1} & 0 & 0 \\ 0 & \Psi & 0 \\ 0 & 0 & I_{\overline{m}-\ell-t+1} \end{bmatrix}^\mathsf{T} \left[\ \Sigma \mid U^\mathsf{T} A_{11}\ \right] \left[\begin{array}{ccc|c} I_{\ell-1} & 0 & 0 & 0 \\ 0 & \Psi & 0 & 0 \\ 0 & 0 & I_{\overline{d}-\ell-t+1} & 0 \\ \hline 0 & 0 & 0 & I_{\overline{n}} \end{array}\right] = \left[\begin{array}{c|c} & u_1^\mathsf{T} A_{11} \\ & \vdots \\ & u_{\ell-1}^\mathsf{T} A_{11} \\ \Sigma & \clubsuit \\ & 0_{t-\tau,\overline{n}} \\ & u_{\ell+t}^\mathsf{T} A_{11} \\ & \vdots \\ & u_{\overline{m}}^\mathsf{T} A_{11} \end{array}\right];$$

simply because the t-by-t block of Σ multiplied by Ψ^T and Ψ from the left and right, respectively, is effectively scalar matrix $\sigma_\ell(B_1) I_t$. Again we can do such modifications for all multiple singular values, and then again permute all the copies of these singular values corresponding to zero rows down.

This brings us to an algorithm, how to decompose the given core problem to the let say proper part and the maximal degenerated subproblem. By the *'properness'* of the first part we mean that it does not contain any further nontrivial degenerated subproblem. This algorithm proceeds as follows (written in pseudo-code and assuming exact arithmetic):

```
Compute the standard SVD of $B_1$, i.e., $B_1 = U\Sigma V^\mathsf{T}$.
Compute $U^\mathsf{T} A_{11}$.
Do (5.27) for all blocks corresponding to multiple singular values.
Find indices $\ell$ ($1 \le \ell \le \overline{d}$) of all zero rows in modified matrix $U^\mathsf{T} A_{11}$.
Remove rows with indices $\ell$ from modified $U^\mathsf{T} A_{11}$, what remains is $A_{11,\alpha}$.
Remove rows and columns with indices $\ell$ from $\Sigma$, what remains is $B_{1,\alpha}$.
Form a diagonal matrix from the removed singular values to get $B_{1,\beta}$.
```

Remark 2. *Note that the core problem revealing transformation of a problem* $[B, A]$ *(5.10) with full column rank* B *has the (slightly simpler) form*

$$P^{\mathsf{T}} \left[\begin{array}{cc} B & A \end{array} \right] \left[\begin{array}{cc} R & 0 \\ 0 & Q \end{array} \right] = \left[\begin{array}{c|cc} B_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{array} \right].$$

Extracting the maximal degenerated subproblem from the core problem $[B_1, A_{11}]$ *(5.25) has the form*

$$P_1^{\mathsf{T}} \left[\begin{array}{cc} B_1 & A_{11} \end{array} \right] \left[\begin{array}{cc} R_1 & 0 \\ 0 & Q_1 \end{array} \right] = \left[\begin{array}{cc|c} B_{1,\alpha} & 0 & A_{11,\alpha} \\ 0 & B_{1,\beta} & 0 \end{array} \right].$$

One could easily spot an analogy in structures of blocks in both equalities. The only difference seems to be the exchanged roles of the system matrix and right-hand side.

5.3.4 Step IV: Note on decomposition of the degenerated component $[B_{1,\beta}, 0_{\overline{m},0}]$

Now we decompose the degenerated core problem

$$\left[\begin{array}{cc} B_{1,\beta} & 0_{\overline{m}_\beta,0} \end{array} \right],$$

which is similar to the decomposition of the core problem complement (see Section 5.3.2). It is so simply because of the analogy mentioned in the last remark. But now the decomposition is even simpler because $[B_{1,\beta}, 0_{\overline{m}_\beta,0}] = B_{1,\beta}$ is the square invertible matrix. Thus, we get

$$\left[\begin{array}{cc} B_{1,\beta} & 0_{\overline{m}_\beta,0} \end{array} \right] \sim \left(\boxplus_{\ell=1}^{\overline{m}_\beta} \left[\begin{array}{cc} \sigma_\ell(B_{1,\beta}) & 0_{1,0} \end{array} \right] \right). \tag{5.28}$$

5.3.5 Step V: Decomposing the proper part of core problem $[B_{1,\alpha}, A_{11,\alpha}]$ — examples of irreducible core problems

Till this moment we did all the easy job. It remains to analyze possible decomposability of the proper core problem $[B_{1,\alpha}, A_{11,\alpha}]$ (i.e., such core problem that already does not contain any degenerated component). We know that it has some finite irreducible representation due to the strict decrease of the quantity (5.20) while decomposing. However, this question seems to be still very difficult to answer.

We start with the description of core problems that are clear or known for being irreducible. There are two specific classes of irreducible core problems:

- Incompatible single right-hand side CPs ($\overline{m} = \overline{n} + 1$ and $\overline{d} = 1$)

$$\left[\begin{array}{cc} B_{1,\alpha} & A_{11,\alpha} \end{array}\right] \sim \left[\begin{array}{c|cccc} b_{11} & \sigma_1 & & & \\ b_{21} & & \sigma_2 & & \\ \vdots & & & \ddots & \\ b_{\overline{n},1} & & & & \sigma_{\overline{n}} \\ b_{\overline{n}+1,1} & 0 & 0 & \dots & 0 \end{array}\right] \sim \left[\begin{array}{c|ccccc} \varphi_1 & \psi_1 & & & & \\ & \varphi_2 & \psi_2 & & & \\ & & \ddots & \ddots & & \\ & & & & \varphi_{\overline{n}} & \psi_{\overline{n}} \\ & & & & & \varphi_{\overline{n}+1} \end{array}\right],$$

  where $b_{t,1} \neq 0$ for all ts and $\sigma_1 > \sigma_2 > \ldots > \sigma_{\overline{n}} > 0$ in the first, and $\varphi_t > 0$, $\psi_t > 0$ for all ts in the second representation.
- Compatible single right-hand side CPs ($\overline{m} = \overline{n}$ and $\overline{d} = 1$)

$$\left[\begin{array}{cc} B_{1,\alpha} & A_{11,\alpha} \end{array}\right] \sim \left[\begin{array}{c|cccc} b_{11} & \sigma_1 & & & \\ b_{21} & & \sigma_2 & & \\ \vdots & & & \ddots & \\ b_{\overline{n},1} & & & & \sigma_{\overline{n}} \end{array}\right] \sim \left[\begin{array}{c|ccccc} \varphi_1 & \psi_1 & & & \\ & \varphi_2 & \psi_2 & & \\ & & \ddots & \ddots & \\ & & & \varphi_{\overline{n}} & \psi_{\overline{n}} \end{array}\right],$$

  where $b_{t,1} \neq 0$ for all ts and $\sigma_1 > \sigma_2 > \ldots > \sigma_{\overline{n}} > 0$ in the first, and $\varphi_t > 0$, $\psi_t > 0$ for all ts in the second representation.

In both cases the irreducibility follows immediately from the fact that $\overline{d} = 1$. Clearly, nonnegative integer partitioning of $\overline{d} = \overline{d}_\alpha + \overline{d}_\beta$ always yields one $\overline{d}_j = 0$, i.e., the jth component is degenerated with empty right-hand side, i.e., it is fully degenerated (see Table 5.2). Therefore, any decomposition of such problems would be trivial $[B_1, A_{11}] = [B_1, A_{11}] \boxplus [0_{0,0}, 0_{0,0}]$, but we are interested only in the nontrivial decompositions. (Note that these two representations are originated in the core problem revealing by the SVD of the system matrix, and by the (generalized) Golub–Kahan iterative bidiagonalization; see [22].)

The straightforward question, whether there exist irreducible core problems with $\overline{d} > 1$, was positively answered in [4, Exampe 4.5], where it is shown that

$$\left[\begin{array}{cc} B_{1,\alpha} & A_{11,\alpha} \end{array}\right] = \frac{1}{4}\left[\begin{array}{cccc} 3 & & & \\ & 2 & & \\ & & 2 & \\ & & & 1 \end{array}\right]\left[\begin{array}{cc|cc} -1 & 3 & \sqrt{3} & \sqrt{3} \\ -3 & -1 & \sqrt{3} & -\sqrt{3} \\ \sqrt{3} & \sqrt{3} & 1 & -3 \\ \sqrt{3} & -\sqrt{3} & 3 & 1 \end{array}\right]$$

is actually the core problem and it is irreducible. The irreducibility is there proven by exhausting all possibilities, i.e., essentially by considering all possible dimensions of potential subproblems and searching the whole corresponding orthogonal group.

Clearly, this approach can be applied also to other particular problems (with concrete numbers) with similar structure (i.e., having the same dimensions, the same multiplicities of singular values, etc.). However, it seems that the analysis of such problem with similar structure is untreatable in general.

Consequently, we leave questions of decomposability of proper core problems, and of characterization of general proper irreducible core problem open. We are going to focus on them in future research.

5.3.6 Summary of steps I–V

In steps (particularly) I–IV we have shown, that for any $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times d}$, there exist orthogonal matrices $P' \in \mathbb{O}_m$, $Q' \in \mathbb{O}_m$, $R' \in \mathbb{O}_m$, such that

$$
P'^{\mathsf{T}} \begin{bmatrix} B & A \end{bmatrix} \begin{bmatrix} R' & 0 \\ 0 & Q' \end{bmatrix} = \left[\begin{array}{ccc|cc} B_{1,\alpha} & 0 & 0 & A_{11,\alpha} & 0 \\ 0 & B_{1,\beta} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & A_{22} \end{array}\right],
$$

where

- the proper core problem $A_{11,\alpha}$, B_1 is of minimal dimensions,
- the degenerated core problem right-hand side matrix $B_{1,\beta}$ is of maximal dimensions and square invertible,
- and the core problem complement system matrix A_{22} is of maximal dimensions.

In the terms of decomposition (see (5.21), (5.24), (5.28), (5.22), and (5.23))

$$
\begin{array}{l}
\left.\begin{array}{l}
\begin{bmatrix} B & A \end{bmatrix} \sim \begin{bmatrix} B_{1,\alpha} & A_{11,\alpha} \end{bmatrix} \\[1em]
\qquad \boxplus \left(\mathop{\boxplus}\limits_{\ell=1}^{\overline{m}_\beta} \begin{bmatrix} \sigma_\ell(B_{1,\beta}) & 0_{1,0} \end{bmatrix} \right)
\end{array}\right\} \text{the core problem} \\[1em]
\left.\begin{array}{l}
\qquad \boxplus \begin{bmatrix} 0_{0,d-\overline{d}} & 0_{0,0} \end{bmatrix} \\[1em]
\qquad \boxplus \left(\mathop{\boxplus}\limits_{\ell=1}^{\min(m-\overline{m},n-\overline{n})} \begin{bmatrix} 0_{1,0} & \sigma_\ell(A_{22}) \end{bmatrix} \right) \\[1em]
\qquad \boxplus \begin{cases} \begin{bmatrix} 0_{(m-\overline{m})-(n-\overline{n}),0} & 0_{(m-\overline{m})-(n-\overline{n}),0} \end{bmatrix} & \text{if } m-\overline{m} > n-\overline{n} \\ \begin{bmatrix} 0_{0,0} & 0_{0,0} \end{bmatrix} & \text{if } m-\overline{m} = n-\overline{n} \\ \begin{bmatrix} 0_{0,0} & 0_{0,(n-\overline{n})-(m-\overline{m})} \end{bmatrix} & \text{if } m-\overline{m} < n-\overline{n} \end{cases}
\end{array}\right\} \text{the core problem complement}
\end{array}
$$

We also know, that the proper core problem $[B_{1,\alpha}, A_{11,\alpha}]$ can be further decomposed and this decomposition is finite.

5.4 NOTE ON TLS SOLVABILITY IN THE CONTEXT OF COMPOSITIONS

Finally, we would like to briefly note on the TLS solvability in the context of (core) problem (de)composition. The most important results in this direction are mentioned in papers [5], [4], and [10] (the copy of the latest one follows this section).

The TLS minimization is orthogonally invariant, which is why we are working with orthogonally equivalent classes of problems, but it is not composition invariant. In particular, the core problem reduction more-or-less commutes with the TLS minimization (up to the '*detail*' that it has to be replaced by the non-generic approach for problems from classes $\mathcal{F}_2$, $\mathcal{F}_3$, and $\mathcal{S}$); see Section 1.2 and papers [5] and [4]. However, as a consequence, the basic decomposition to the core problem and the core problem complement is always useful when searching for the TLS solution. That is so simply because the core problem complement system matrix A_{22} can always be ignored in the minimization as it has no impact on the solution anyway.

On the other hand, the decomposition of the core problem itself and the TLS minimization does not commute at all: TLS minimization is essentially driven by the singular values of the extended matrix $[B, A]$, i.e., when applied on the composed problem, it deals with all the components at the same time, in general. Respectively, it depends on the mutual distribution of singular values of the individual components — but this might be completely random, especially when the components are in some real-world problem originated in completely different uncorrelated phenomenons. This may result, e.g., in full damping or regularizing-out some components with sufficiently small singular values (and consequently the norm; in comparison to other components); see [4, Example 5.3]. The other way summarized by:

First decompose, then solve, and finally compose solutions

may therefore end up with completely different answers; see [4] and [10].

Two of the previous results or observations may be, however, useful in the context of this '*first decompose, then solve*' reasoning:

- The degenerated subproblem $[B_{1,\beta}, 0_{\overline{m}_\beta,0}]$ within the core problem (see Section 5.3.3) represents a '*pure residuum*'. There is clearly no way to approximate the square invertible matrix $B_{1,\beta}$ by columns of zero (moreover empty) system matrix $0_{\overline{m}_\beta,0}$. The only available choice for the corresponding approximate solution clearly is the empty (and thus also zero) matrix $0_{0,\overline{m}_\beta}$.
- On the other side of solvability spectrum, there are the compatible components within the proper core problem (see the second class of irreducible core problems in Section 5.3.5). Such problems can be solved in the classical sense. Consequently, contrary to the previous item, these problems do not contribute to the residuum at all. Moreover, since such problem is still the core problem (satisfying in particular (CP1) and (CP4) properties), its system matrix is always square invertible and, thus, its solution is always unique.

How such subproblems affect the TLS solution of a composed problem, while solving it at once (i.e., not component-wisely), is not fully clear. As already mentioned, it is strongly influenced by the interplay of singular values of the individual components. The analysis of such interplay of several components w.r.t. the TLS solvability was preliminarily studied in particular in our paper [10]; see the included copy at page 83.

MAJOR PUBLISHED RESULTS RELATED TO THE PART II

1. I. Hnětynková, M. Plešinger, and J. Žáková, *Solvability classes for core problems in matrix total least squares minimization*, Applications of Mathematics 64 (2) (2019), pp. 103–128.

   `https://link.springer.com/article/10.21136/am.2019.0252-18`

   See also page 83, or reference [10].

64 (2019) APPLICATIONS OF MATHEMATICS No. 2, 103–128

SOLVABILITY CLASSES FOR CORE PROBLEMS IN MATRIX TOTAL LEAST SQUARES MINIMIZATION

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Received September 20, 2018. Published online February 19, 2019.

Abstract. Linear matrix approximation problems $AX \approx B$ are often solved by the total least squares minimization (TLS). Unfortunately, the TLS solution may not exist in general. The so-called core problem theory brought an insight into this effect. Moreover, it simplified the solvability analysis if B is of column rank one by extracting a core problem having always a unique TLS solution. However, if the rank of B is larger, the core problem may stay unsolvable in the TLS sense, as shown for the first time by Hnětynková, Plešinger, and Sima (2016). Full classification of core problems with respect to their solvability is still missing. Here we fill this gap. Then we concentrate on the so-called composed (or reducible) core problems that can be represented by a composition of several smaller core problems. We analyze how the solvability class of the components influences the solvability class of the composed problem. We also show on an example that the TLS solvability class of a core problem may be in some sense improved by its composition with a suitably chosen component. The existence of irreducible problems in various solvability classes is discussed.

Keywords: linear approximation problem; core problem theory; total least squares; classification; (ir)reducible problem

MSC 2010: 15A06, 15A09, 15A18, 15A23, 65F20

1. Introduction

1.1. The core problem theory. Let us consider a *linear approximation problem*

$$AX \approx B, \quad \text{where } A \in \mathbb{R}^{m\times n},\ B \in \mathbb{R}^{m\times d},\ X \in \mathbb{R}^{n\times d} \tag{1.1}$$

are matrices representing the system matrix of a discretized model, observation ma-

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The research of Iveta Hnětynková has been supported by the GAČR grant No. GA17-04150J. The research of Martin Plešinger and Jana Žáková has been supported by the SGS grant of Technical University of Liberec No. 21254/2018.

DOI: 10.21136/AM.2019.0252-18

trix of measurements (together forming the data matrix $[B, A]$), and the matrix of unknowns, respectively. For simplicity we usually assume $\mathcal{R}(B) \not\subseteq \mathcal{R}(A)$ and $\mathcal{R}(B) \not\subseteq \mathcal{N}(A^{\mathrm{T}})$, otherwise the problem has either a solution in a classical sense $AX = B$ with $X \equiv A^{\dagger}B$, or the column spaces of both matrices are orthogonal $A^{\mathrm{T}}B = 0$ and it makes no sense to approximate columns of B by columns of A, (where $\mathcal{R}(K)$, $\mathcal{N}(K)$, and $K^{\dagger}$ denote respectively the range, null-space, and Moore–Penrose pseudoinverse of K).

The *core problem theory* developed in [8], [4], [5] gives the following. For every (1.1), there exist orthogonal matrices $P \in \mathbb{R}^{m\times m}$, $P^{\mathrm{T}} = P^{-1}$, $Q \in \mathbb{R}^{n\times n}$, $Q^{\mathrm{T}} = Q^{-1}$, $R \in \mathbb{R}^{d\times d}$, $R^{\mathrm{T}} = R^{-1}$ so that

$$(P^{\mathrm{T}}AQ)(Q^{\mathrm{T}}XR) \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \approx \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix} \equiv (P^{\mathrm{T}}BR), \tag{1.2}$$

with conforming partitioning of matrices (i.e., in particular, A_{11} and B_1 have the same number of rows) satisfying the following three conditions:

(CP1) The matrix A_{11} is of *full column rank.*

(CP2) The matrix B_1 is of *full column rank.*

(CP3) Let A_{11} have ξ distinct nonzero singular values with multiplicities μ_j and $\mu_{\xi+1} \equiv \dim(\mathcal{N}(A_{11}^{\mathrm{T}}))$, and let U'_j be matrices having orthonormal bases of left singular vector subspaces of A_{11} as their columns.
The matrix $(U'_j)^{\mathrm{T}}B_1$ is of *full row rank* μ_j for $j = 1, \ldots, \xi, \xi + 1$.

In [8] and [4], it was shown, that (CP1)–(CP3) are equivalent to the minimality of $[B_1, A_{11}]$ (and maximality of A_{22}) over all orthogonal transformations giving the same zero-nonzero block structure of the system and observation matrices. Note that [8] focuses on the case $d = 1$, i.e., when B and therefore also B_1 are vectors, while [4] focuses on the matrix right-hand side case $d > 1$. The minimally dimensioned subproblem

$$A_{11}X_{11} \approx B_1 \tag{1.3}$$

is called the *core problem* (within (1.1)) and (1.2) is the *core problem revealing transformation.*

1.2. The total least squares minimization. Problems of the form (1.1) are solved in many applications by using plenty of different approaches, usually based on least squares techniques. Total least squares (TLS) minimization represents one of them. It typically seeks for

$$\min_{G\in\mathbb{R}^{m\times d},\, E\in\mathbb{R}^{m\times n}} \|[G, E]\|_F \quad \text{subject to } \mathcal{R}(B + G) \subseteq \mathcal{R}(A + E) \tag{1.4}$$

(where $\|K\|_F$ denotes the Frobenius norm of K). Then any matrix X^{TLS} satisfying

$$(A+E)X^{\mathrm{TLS}} = B+G$$

is called the TLS solution of (1.1).

The TLS problem differs from the basic (ordinary) LS in including a correction E of the model matrix A into the minimization formulation. Problems, for which a TLS solution represents better approximation than a LS solution have been widely discussed in the literature in the past decades. A nice overview can be found, e.g., in [10], Chapter 1.2 or [7]. For example, the TLS approach is advantageous in classical errors-in-variables (EIV) models, where the aim is to reveal the existing unknown model (representing relations between variables) from its approximation A rather than obtaining a precise approximation of X, or in cases where model errors are significantly larger than observation errors. The TLS method is applied (under various names) in areas such as experimental modal analysis, system identification, signal processing, image processing or chemometrics, see [7] for references, where LS often fails to give reliable approximations.

However, allowing corrections of A in (1.4) has significant impact on the solvability of the minimization problem. While LS solution always exists (and one can uniquely select a solution with minimum norm), this is no longer true for TLS. The existence and uniqueness of X^{TLS} has been analyzed in many papers starting from [1], [10], [12], [13], and in particular [14]. Moreover, the so-called nongeneric solution was defined in [10] for cases where the standard TLS solution does not exist or is complicated to construct (as revealed and explained later in [3]). The question of TLS solvability of a general problem (1.4) was finally resolved in [14] and [3]. In particular, [3] introduced a novel full classification of problems (1.1) with respect to their TLS solvability. The problems (1.1) are there divided into four *solvability classes* and for each of them the (non)existence and (non)uniqueness of the TLS solution is proved. Thus, the solvability class of a given problem reveals how its approximate solution can be computed, and what is the meaning of this solution in terms of the original data.

The TLS minimization (1.4) employs the Frobenius, i.e., orthogonally invariant norm, and the core problem revealing transformation (1.2) is an orthogonal transformation. Thus the TLS minimizations applied to the original and transformed problems result in the same minima (up to the transformation). Taking into account the zero blocks in the transformed right-hand side (1.2), it is reasonable to put $X_{12}=0$, $X_{21}=0$, $X_{22}=0$. Consequently, using the core reduction as a sort of preprocessing of the data A, B, it is obvious that we in fact need to solve the single nontrivial and typically smaller subproblem—the core problem (1.3). The link between the TLS solution of the core problem and the TLS or non-generic solution of the original problem if $d = 1$ was explained in [8]. There it was also proved that the core problem with $d = 1$ is always uniquely TLS solvable. For problems with $d > 1$, the first attempts of clarification were published in [2]. In particular it was shown that if $d > 1$, the *core problem may stay unsolvable* in the TLS sense. However, complete classification of core problems with respect to their solvability is still missing. Such knowledge would indicate in which cases the core reduction simplifies the solvability of the TLS problem, and clarify the meaning of the TLS solution of the core problem with respect to the original data. Thus we study this open question here.

1.3. Contribution of this work. In this paper we present some further pieces of the missing mosaic. We show which solvability classes are possible for core problems with $d = 2$ and $d > 2$, resulting in *full solvability classification of core problems* with respect to the number of their right-hand sides. Then we concentrate on the so-called *composed (or reducible) core problems* introduced in [2]. Such problems can be equivalently represented by a composition of several (in some sense block independent) core problems of smaller dimensions. Assuming the solvability classes of the components are known, we analyze feasible solvability classes of the resulting composed problem. We also show on an example that the TLS solvability of a core problem may be in some sense improved by its composition with a suitably chosen component. For completeness, examples of irreducible problems in various solvability classes are presented.

The text is organized as follows. Section 2 recapitulates the TLS classification, the previous TLS solvability results for core problems, and the core problem composition. Section 3 gives the full solvability classification of core problems with respect to the number of their right-hand sides. Section 4 analyzes solvability classes in the course of core problems composing. Section 5 comments on the irreducible core problems, and Section 6 concludes the paper.

2. Recapitulation of known results

2.1. Classification of TLS problems. First of all we briefly recall the above-mentioned full classification of problems with respect to their TLS solvability developed in [3]. It employs the singular value decompositions (SVD) of the data matrix $[B, A] \in \mathbb{R}^{m\times(n+d)}$ (we assume $m \geqslant n + d$ for simplicity; in the other case one can add zero rows to the data matrix, which is equivalent to adding $(n + d) - m$ zero singular values). Let

$$[B, A] = U\Sigma V^{\mathrm{T}}, \quad \text{where } \Sigma = \begin{bmatrix} \mathrm{diag}(\sigma_1, \ldots, \sigma_{n+d}) \\ 0 \end{bmatrix} \in \mathbb{R}^{m\times(n+d)}, \tag{2.1}$$

let q ($0 \leqslant q \leqslant n$) and e ($1 \leqslant e \leqslant d$) be the *left-* and *right-multiplicity* of σ_{n+1}, e.g.,

$$\sigma_{n-q} > \underbrace{\sigma_{n-q+1} = \ldots = \sigma_{n+1} = \ldots = \sigma_{n+e}}_{(q+e)\text{-tuple singular value}} > \sigma_{n+e+1} \tag{2.2}$$

in the typical case (if $q = n$ or $e = d$, then σ_{n-q} or σ_{n+e+1} do not exist, respectively). The classification is then based on ranks of individual blocks of V,

$$V = \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} \begin{matrix} \}\, d \\ \}\, n \end{matrix} = \begin{bmatrix} V_{11} & V_{12} & V_{13} \\ V_{21} & V_{22} & V_{23} \end{bmatrix} \begin{matrix} \}\, d \\ \}\, n \end{matrix} \tag{2.3}$$
$$\qquad\qquad\qquad \underbrace{\quad}_{n-q} \underbrace{\quad}_{q+e} \underbrace{\quad}_{d-e}$$

(if $q = n$ or $e = d$, then $[V_{11}^{\mathrm{T}}, V_{21}^{\mathrm{T}}]^{\mathrm{T}}$ or $[V_{13}^{\mathrm{T}}, V_{23}^{\mathrm{T}}]^{\mathrm{T}}$ have no columns, respectively). Then (1.1) with the minimization (1.4) belongs to the class:

- $\mathcal{F}$ if $\operatorname{rank}([V_{12}, V_{13}]) = d$ (so-called *generic* problem), in particular to its sub-class:
  - $\mathcal{F}_1$ if $\operatorname{rank}(V_{12}) = e$,
  - $\mathcal{F}_2$ if $\operatorname{rank}(V_{12}) > e$ and $\operatorname{rank}(V_{13}) = d - e$, or
  - $\mathcal{F}_3$ if $\operatorname{rank}(V_{13}) < d - e$ (i.e., $\mathcal{F} = \mathcal{F}_1 \cup \mathcal{F}_2 \cup \mathcal{F}_3$); or
- $\mathcal{S}$ if $\operatorname{rank}([V_{12}, V_{13}]) < d$ (so-called *non-generic* problem).

The problem has a TLS solution if and only if it belongs to $\mathcal{F}_1 \cup \mathcal{F}_2$, as shown in [3]. Thus problems in $\mathcal{F}_3 \cup \mathcal{S}$ (i.e., even the generic problems in $\mathcal{F}_3$) have no TLS solution. This classification has been recently extended to TLS formulations with an arbitrary unitarily invariant norm in (1.4), see [11].

Note that the so-called *classical TLS algorithm* (see [10], [3]) returns the TLS solution only for problems from $\mathcal{F}_1$, moreover it always returns the solution minimal in both the Frobenius and spectral norms. For problems from $\mathcal{F}_2$, the algorithm requires a small modification (see [6]), but it is not able to return the minimal norm solution in general.

2.2. Solvability of core problems. The key result proved in [8] for $d = 1$ is the following: The core problem with single right-hand side has always the unique TLS solution X_{11}^{TLS}. Moreover, its back-transformation $X = Q\left[(X_{11}^{\mathrm{TLS}})^{\mathrm{T}}, 0\right]^{\mathrm{T}} R^{\mathrm{T}}$ (since $d = 1$, R becomes equal to 1 or -1) is the (unique or minimum norm) TLS solution of the original problem (if it is TLS solvable), or the so-called (unique or minimum norm) nongeneric solution (otherwise).

In the context of solvability classification, it was shown in [3] that a problem $AX \approx B$ with a single right-hand side belongs either to $\mathcal{F}_1$ or $\mathcal{S}$, and the core problem $A_{11}X_{11} \approx B_1$ with a single right-hand side belongs always to $\mathcal{F}_1$. (Recall that all problems in $\mathcal{F}_1$ are TLS solvable, whereas in $\mathcal{S}$ they are not.) Note that in [2] it was also shown that *any core problem* (i.e., with $d = 1$ as well as $d > 1$) in $\mathcal{F}_1$ has a *unique TLS solution.*

Since the solution of the original problem and the core problem within are closely linked, authors of [8] say that for $d = 1$ the core problem contains *only the necessary and all the sufficient information* for solving the original problem in the TLS sense. Therefore, the transition from the original general problem (GP) to the core problem (CP) is called the *core problem reduction.* To simplify the exposition, we schematically describe this by the diagram:

$$(\mathsf{GP}, 1, \mathcal{F}_1 \text{ or } \mathcal{S}) \xrightarrow[\text{reduction}]{\text{core problem}} (\mathsf{CP}, 1, \mathcal{F}_1), \tag{2.4}$$

where the first component of each triplet identifies whether we deal with general or core problem, the second component specifies the number of its right-hand sides d, and the last component denotes its solvability class. In the general case $d \geqslant 1$, such scheme takes the form:

$$(\mathsf{GP}, d, \text{any class}) \xrightarrow[\text{reduction}]{\text{core problem}} (\mathsf{CP}, \overline{d}, \text{unknown class}), \quad d \geqslant \overline{d} \geqslant 1, \tag{2.5}$$

since nothing is known about the resulting class of the core problem.

2.3. Composing of core problems. In [2], it was shown that we can *compose the core problems* as follows. If $A_{11}^{(l)} X_{11}^{(l)} \approx B_1^{(l)}$, $l = \alpha, \beta$, represent two core problems (i.e., each satisfies (CP1)–(CP3)), then the problem

$$A_{11} X_{11} \equiv \left(P^{\mathrm{T}} \begin{bmatrix} A_{11}^{(\alpha)} & 0 \\ 0 & A_{11}^{(\beta)} \end{bmatrix} Q \right) X_{11} \approx \left(P^{\mathrm{T}} \begin{bmatrix} B_1^{(\alpha)} & 0 \\ 0 & B_1^{(\beta)} \end{bmatrix} R \right) \equiv B_{11}, \tag{2.6}$$

where P, Q, R are orthogonal matrices, also satisfies (CP1)–(CP3) and therefore represents a core problem. We call such a core problem *composed or reducible.* Schematically, we describe the composition by the sign "$\boxplus$" with the particular summands indexed by small Greek letters from the beginning of the alphabet.

The relationship between $X_{11}^{(\alpha)}$, $X_{11}^{(\beta)}$, and X_{11} is not clear, except for some special cases. In particular, it was shown by examples in [2] that there *exist two components* such that

$$(\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta = (\mathsf{CP}, 2, \mathcal{F}_1) \text{ or } (\mathsf{CP}, 2, \mathcal{F}_2) \text{ or } (\mathsf{CP}, 2, \mathcal{S}). \tag{2.7}$$

Further, there *exist three components* such that

$$(\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma = (\mathsf{CP}, 3, \mathcal{F}_3). \tag{2.8}$$

Thus the core problem with $d > 1$ can belong to any of the four solvability classes. Note that not every core problem with $d > 1$ can be written as a composition of single right hand-side core problems. In [2], an example of irreducible $\mathcal{F}_2$ core problem was presented.

Even though we have excluded compatible problems (i.e., with $\mathcal{R}(B) \subseteq \mathcal{R}(A)$) and "fully incompatible" problems (i.e., with $\mathcal{R}(B) \subseteq \mathcal{N}(A^{\mathrm{T}})$, or equivalently $\mathcal{R}(B) \perp \mathcal{R}(A)$ or $A^{\mathrm{T}}B = 0$), a component of a core problem can still have such properties. If we try to find the core problem within a fully incompatible problem, we see that B_1 is square invertible, and formally A_{11} has no columns, i.e., the data matrix takes the form $[B_1, A_{11}] = B_1$. Such *degenerated core problem* can play a role of a component (which cannot be approximated and only increases the residual) in a composed problem. The degenerated component is always of $\mathcal{F}_1$. For illustration, we give examples of the *proper incompatible*, *compatible*, and *degenerated core problems* (or their components) $A_{11}X_{11} \approx B_1$, $A_{11} \in \mathbb{R}^{m\times n}$, $B_1 \in \mathbb{R}^{m\times d}$, with $d = 1$. Their so-called *SVD forms* always look like

$$[B_1, A_{11}] = \left[\begin{array}{c|cccc} b_1 & \varsigma_1 & & & \\ b_2 & & \varsigma_2 & & \\ \vdots & & & \ddots & \\ b_n & & & & \varsigma_n \\ b_{n+1} & 0 & 0 & \dots & 0 \end{array}\right], \quad \left[\begin{array}{c|cccc} b_1 & \varsigma_1 & & & \\ b_2 & & \varsigma_2 & & \\ \vdots & & & \ddots & \\ b_n & & & & \varsigma_n \end{array}\right], \quad \text{and} \quad [\,b_1\,],$$

respectively, where $b_j \neq 0$ and $\varsigma_j > \varsigma_{j+1} > 0$. Clearly $m = n + 1$, n, and 1 in these three respective cases, and $n = 0$ in the last one.

3. Solvability classes of core problems with respect to the number of their right-hand sides

The single right-hand side core problem always belongs to the class $\mathcal{F}_1$, see [8]. Examples of $\mathcal{F}_2$, and $\mathcal{S}$ core problems are in (2.7) built up from two single right-hand components, whereas $\mathcal{F}_3$ core problem in (2.8) is built up from three, see [2]. This motivates a question whether the number of right-hand sides d restricts the available classes of core problems not only for $d = 1$ but also for $d > 1$. We analyze this below.

3.1. Core problems with two right-hand sides. The following theorem gives all possible classes for $d = 2$.

Theorem 3.1. *Let $A_{11}X_{11} \approx B_1$, $B_1 \in \mathbb{R}^{m\times d}$, be a core problem with $d = 2$ right-hand sides. Then the core problem belongs to the class $\mathcal{F}_1$, $\mathcal{F}_2$, or $\mathcal{S}$. Equivalently, the core problem with $d = 2$ cannot belong to the class $\mathcal{F}_3$.*

Proof. Recalling that there exist composed core problems with $d = 2$ in $\mathcal{F}_1$, $\mathcal{F}_2$, and $\mathcal{S}$ (see (2.7)), we only need to exclude $\mathcal{F}_3$.

Assume by contradiction that there exists a core problem with $d = 2$ in $\mathcal{F}_3$. The classification is based on the ranks of blocks of V (see (2.3)), and the class $\mathcal{F}_3$ is characterized by $\operatorname{rank}([V_{12}, V_{13}]) = d$ and $\operatorname{rank}(V_{13}) < d - e$, where e $(1 \leqslant e \leqslant d)$ is the right-multiplicity of the singular value σ_{n+1}. Since $d = 2$, we have $e \in \{1, 2\}$. The inequality $\operatorname{rank}(V_{13}) < d - e = 2 - e$ then implies that

$$e = 1, \quad \operatorname{rank}(V_{13}) = 0, \quad \text{and} \quad V_{13} \in \mathbb{R}^{2\times 1}. \tag{3.1}$$

Because the number of columns of V_{13} is equal to the sum of multiplicities of singular values strictly smaller than σ_{n+1}, we see that there is only one simple (possibly zero) singular value with this property, i.e., $\sigma_{n+1} > \sigma_{n+2} \geqslant 0$. Here we need to use another property of core problems that has not been mentioned yet:

(CP5) Let $[B_1, A_{11}]$ have χ distinct nonzero singular values with multiplicities ϱ_j and $\varrho_{\chi+1} \equiv \dim(\mathcal{N}([B_1, A_{11}]))$, and let V'_j be matrices having orthonormal bases of left singular vector subspaces of $[B_1, A_{11}]$ as their columns.
The leading $d \times \varrho_j$ submatrix of V'_j is of *full column rank* ϱ_j for $j = 1, \ldots, \chi, \chi + 1$; see [5] and [2].

We see that $[V_{13}^{\mathrm{T}}, V_{23}^{\mathrm{T}}]^{\mathrm{T}}$ is one of the matrices V'_j, and V_{13} is one of the $d \times \varrho_j$ blocks. Therefore, V_{13} has linearly independent columns, i.e., is of rank one which is in contradiction with (3.1). □

Note that in the case of composed core problem (i.e., having two single right-hand side components), this theorem directly implies that, schematically:
$\forall(\mathsf{CP}, 1, \mathcal{F}_1)_\alpha$, $\forall(\mathsf{CP}, 1, \mathcal{F}_1)_\beta$,

$$(\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta = (\mathsf{CP}, 2, \mathcal{F}_1),\ (\mathsf{CP}, 2, \mathcal{F}_2),\ \text{or}\ (\mathsf{CP}, 2, \mathcal{S}),$$

or equivalently

$$(\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta \neq (\mathsf{CP}, 2, \mathcal{F}_3).$$

3.2. Core problems with three and more right-hand sides.

First we prove a theorem stating that it is always possible to compose a general core problem with a single right-hand side component without changing the solvability class.

Theorem 3.2. *Let* $A_{11}^{(\alpha)} X_{11}^{(\alpha)} \approx B_1^{(\alpha)}$, $A_{11}^{(\alpha)} \in \mathbb{R}^{m_\alpha \times n_\alpha}$, $B_1^{(\alpha)} \in \mathbb{R}^{m_\alpha \times d_\alpha}$ *be a core problem (that will serve as a component) and let it be in the class* $\mathcal{C} \in \{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{S}\}$.

Then there exists a single right-hand side component $A_{11}^{(\beta)} X_{11}^{(\beta)} \approx B_1^{(\beta)}$, $A_{11}^{(\beta)} \in \mathbb{R}^{m_\beta \times n_\beta}$, $B_1^{(\beta)} \in \mathbb{R}^{m_\beta \times 1}$ *such that the composed core problem*

$$A_{11} X_{11} \equiv \left(P^{\mathrm{T}} \begin{bmatrix} A_{11}^{(\alpha)} & 0 \\ 0 & A_{11}^{(\beta)} \end{bmatrix} Q \right) X_{11} \approx \left(P^{\mathrm{T}} \begin{bmatrix} B_1^{(\alpha)} & 0 \\ 0 & B_1^{(\beta)} \end{bmatrix} R \right) \equiv B_{11},$$

is also in the class $\mathcal{C}$.

Schematically: $\forall (\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha$, $\exists (\mathsf{CP}, 1, \mathcal{F}_1)_\beta$ such that

$$(\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha + 1, \mathcal{C}),$$

where $\mathcal{C} \in \{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{S}\}$.

Proof. Let $\sigma_i^{(\alpha)}$, $i = 1, \ldots n_\alpha + d_\alpha$, be the singular values of the α-component $[B_1^{(\alpha)}, A_{11}^{(\alpha)}]$. Denote q_l, e_l the left- and right-multiplicity of the singular value of interest, i.e., $\sigma_{n_l+1}^{(\alpha)}$. Construct a core problem representing the β-component $[B_1^{(\beta)}, A_{11}^{(\beta)}]$ arbitrarily with the only restriction that

$$\sigma_{n_\beta+1}^{(\beta)} = \sigma_{n_\alpha+1}^{(\alpha)}.$$

Since $d_\beta = 1$, the singular values of the β-component are simple and thus the left- and right-multiplicity of $\sigma_{n_\beta+1}^{(\beta)}$ is $q_\beta = 0$, $e_\beta = 1$. Then in the partitioning of the $V^{(l)}$ matrix from the SVDs of the extended matrices, we get

$$V_1^{(\alpha)} = [\underbrace{V_{11}^{(\alpha)}}_{n_\alpha - q_\alpha}, \underbrace{V_{12}^{(\alpha)}}_{q_\alpha + e_\alpha}, \underbrace{V_{13}^{(\alpha)}}_{d_\alpha - e_\alpha}] \;\}\; d_\alpha, \quad V_1^{(\beta)} = [\underbrace{V_{11}^{(\beta)}}_{n_\beta}, \underbrace{V_{12}^{(\beta)}}_{1}] \;\}\; 1,$$

here $V_{13}^{(\beta)}$ does not exist (it has zero columns). Moreover, $V_{12}^{(\beta)} = v_{1,n_\beta+1}^{(\beta)} \neq 0$. Then, similarly to (3.3),

$$\begin{aligned} [V_{11}, V_{12}, V_{13}] &= R^{\mathrm{T}} \begin{bmatrix} V_1^{(\alpha)} & 0 \\ 0 & V_1^{(\beta)} \end{bmatrix} \Psi, \\ &= R^{\mathrm{T}} \left[\begin{array}{cc|cc|c} V_{11}^{(\alpha)} & 0 & V_{12}^{(\alpha)} & 0 & V_{13}^{(\alpha)} \\ 0 & V_{11}^{(\beta)} & 0 & V_{12}^{(\beta)} & 0 \end{array} \right] \left[\begin{array}{c|c|c} \Psi_{11} & & \\ \hline & I & \\ \hline & & I \end{array} \right]. \end{aligned}$$

Clearly,

$$\begin{aligned} \operatorname{rank}(V_{12}) &= \operatorname{rank} \left(R^{\mathrm{T}} \begin{bmatrix} V_{12}^{(\alpha)} & 0 \\ 0 & v_{1,n_\beta+1}^{(\beta)} \end{bmatrix} \right) = \operatorname{rank}(V_{12}^{(\alpha)}) + 1, \\ \operatorname{rank}(V_{13}) &= \operatorname{rank} \left(R^{\mathrm{T}} \begin{bmatrix} V_{13}^{(\alpha)} \\ 0 \end{bmatrix} \right) = \operatorname{rank}(V_{13}^{(\alpha)}), \\ \text{and} \quad \operatorname{rank}([V_{12}, V_{13}]) &= \operatorname{rank}([V_{12}^{(\alpha)}, V_{13}^{(\alpha)}]) + 1, \end{aligned}$$

where $V_{12} \in \mathbb{R}^{d\times(q+e)}$, $V_{13} \in \mathbb{R}^{d\times(d-e)}$, $d \equiv d_\alpha + 1$, $d - e = d_\alpha - e_\alpha$ so $e \equiv e_\alpha + 1$, and $q + e = q_\alpha + e_\alpha + 1$ so $q \equiv q_\alpha$. Thus the α-component $[B_1^{(\alpha)}, A_{11}^{(\alpha)}]$ and the composed core problem $[B_1, A_{11}]$ are of the same class. □

Consequently, applying the theorem to examples of core problems with $d = 2$ from [2], see (2.7), we find there exist core problems with $d = 3$ in $\mathcal{F}_1$, $\mathcal{F}_2$ and $\mathcal{S}$. Recalling the example (2.8), we see that for $d = 3$ there exist core problems in all four solvability classes. For $d > 3$, we can proceed analogously giving full solvability classification summarized in Table 1. Note that for any given $d > 1$ and any feasible class, we can find a composed core problem having only single right-hand side components. This result is interesting in view of the fact that any core problem with $d = 1$ belongs to $\mathcal{F}_1$ (the set of problems having always the TLS solution).

d	Classes			
1	$\mathcal{F}_1$	—	—	—
2	$\mathcal{F}_1$	$\mathcal{F}_2$	—	$\mathcal{S}$
3 and more	$\mathcal{F}_1$	$\mathcal{F}_2$	$\mathcal{F}_3$	$\mathcal{S}$

Table 1. Core problem with d right-hand sides belongs to one of the following classes.

3.3. Note on composing identical components. In general, it is not known what is the relation between the class of a composed problem and the classes of its components. Now we show that when a core problem is composed with itself, the solvability class cannot change. The theorem gives another way how to construct composed core problems in selected classes.

Theorem 3.3. *Let $A_{11}X_{11} \approx B_1$ be a core problem. If it is composed of two (or more) identical components $A_{11}^{(\alpha)}X_{11}^{(\alpha)} \approx B_1^{(\alpha)}$, then the core problem and its component belong to the same class.*

Schematically:

$$\forall(\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha,\ (\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha \boxplus (\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha = (\mathsf{CP}, 2d_\alpha, \mathcal{C}),$$

$$\text{and thus also}\quad \boxplus_{i=1}^{k} (\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha = (\mathsf{CP}, kd_\alpha, \mathcal{C}),$$

where $\mathcal{C} \in \{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{S}\}$.

Proof. The statement holds trivially for compatible and degenerated components. Therefore, we focus on the proper incompatible components. Recall that

$$[B_1, A_{11}] = P^{\mathrm{T}} \left[\begin{array}{ccc|ccc} B_1^{(\alpha)} & 0 & 0 & A_{11}^{(\alpha)} & 0 & 0 \\ 0 & \ddots & 0 & 0 & \ddots & 0 \\ 0 & 0 & B_1^{(\alpha)} & 0 & 0 & A_{11}^{(\alpha)} \end{array}\right] \left[\begin{array}{c|c} R & 0 \\ \hline 0 & Q \end{array}\right]$$

$$= P^{\mathrm{T}} \left[\, I_k \otimes B_1^{(\alpha)} \;\middle|\; I_k \otimes A_{11}^{(\alpha)} \,\right] \left[\begin{array}{c|c} R & 0 \\ \hline 0 & Q \end{array} \right],$$

where "⊗" denotes the Kronecker product; $A_{11}^{(\alpha)} \in \mathbb{R}^{m_\alpha \times n_\alpha}$, $B_{11}^{(\alpha)} \in \mathbb{R}^{m_\alpha \times d_\alpha}$, $n \equiv kn_\alpha$, $m \equiv km_\alpha$, and $d \equiv kd_\alpha$. Consider the full SVD $[B_1^{(\alpha)}, A_{11}^{(\alpha)}] = U^{(\alpha)}\Sigma^{(\alpha)}(V^{(\alpha)})^{\mathrm{T}}$ with square $U^{(\alpha)}$ and $V^{(\alpha)}$, with partitionings

$$(3.2) \qquad V^{(\alpha)} = \begin{bmatrix} V_1^{(\alpha)} \\ V_2^{(\alpha)} \end{bmatrix} \begin{matrix} \} \, d_\alpha \\ \} \, n_\alpha \end{matrix}, \quad \text{and} \quad V_1^{(\alpha)} = [\, V_{11}^{(\alpha)},\ V_{12}^{(\alpha)},\ V_{13}^{(\alpha)} \,]$$

as in (2.3). This immediately gives the SVD of the composed problem in the form

$$[B_1, A_{11}] = \underbrace{(P^{\mathrm{T}}(I_k \otimes U^{(\alpha)})\Pi)}_{U} \underbrace{(\Pi^{\mathrm{T}}(I_k \otimes \Sigma^{(\alpha)})\Psi)}_{\Sigma} \underbrace{\left(\left[\begin{array}{c|c} R & 0 \\ \hline 0 & Q \end{array} \right]^{\mathrm{T}} \left[\begin{array}{c} I_k \otimes V_1^{(\alpha)} \\ \hline I_k \otimes V_2^{(\alpha)} \end{array} \right] \Psi \right)^{\mathrm{T}}}_{V},$$

where Π and Ψ are permutation matrices sorting the singular values in the nonincreasing order on the diagonal of Σ. Since the permutations realize the commutation of the Kronecker product

$$\Pi^{\mathrm{T}}(I_k \otimes \Sigma^{(\alpha)})\Psi = \Sigma^{(\alpha)} \otimes I_k,$$

where Σ is square, we have simply $\Pi = \Psi$, see [9]. Note that multiplicities of all singular values are in the composed problem k-times larger than in its component.

Let us focus on V and denote $v_{:,j}^{(\alpha)}$ the jth column of $V_1^{(\alpha)}$. Then we get

$$(3.3) \qquad \begin{aligned} V_1 = [\, V_{11}, V_{12}, V_{13} \,] &= R^{\mathrm{T}}(I_k \otimes V_1^{(\alpha)})\Psi \\ &= R^{\mathrm{T}} \, [\, I_k \otimes v_{:,1}^{(\alpha)}, I_k \otimes v_{:,2}^{(\alpha)}, \ldots, I_k \otimes v_{:,n_\alpha + d_\alpha}^{(\alpha)} \,] \,. \end{aligned}$$

Clearly, the dimensions of V_{ij} in (3.3) are k-times larger than the dimensions of $V_{ij}^{(\alpha)}$ in (3.2). From the structure of the last matrix, and since R is orthogonal, we see that

$$\operatorname{rank}(V_{ij}) = \operatorname{rank}(RV_{ij}) = k \cdot \operatorname{rank}(V_{ij}^{(\alpha)}),$$

i.e., also the ranks of V_{ij} are k-times larger than the ranks of $V_{ij}^{(\alpha)}$.

Since the solvability classification is based on multiplicities of singular values, ranks and sizes of the blocks (in particular on the relations between these quantities), and all these quantities are in the composed problem just k-times larger, the component and the composed problem must belong to the same class. □

Theorems 3.2 and 3.3 formulate basic relations between solvability classes in the course of core problems composing in two special cases. Further results are given in the next section.

In all cases discussed previously (see Theorems 3.2 and 3.3, and examples (2.7)), a composition of core problems leads to a composed problem with the same or worse TLS solvability on the scale

$$\mathcal{F}_1 \text{ (the best)}—\mathcal{F}_2—\mathcal{F}_3—\mathcal{S} \text{ (the worst)}.$$

Recall that $\mathcal{F}_1$ problems always have a TLS solution (that can be computed by the classical TLS algorithm), and core problems have a unique TLS solution; $\mathcal{F}_2$ problems also have a TLS solution (that cannot be simply computed by the classical TLS algorithm); $\mathcal{F}_3$ problems are still generic, but they have no TLS solution; and $\mathcal{S}$ problems are nongeneric and have no TLS solution. Such scale naturally corresponds to “removing the linear independence” from the upper right corner of V (see (2.3) and the classification below) and motivates the question whether the composition always worsens the TLS solvability. First we build up an illustrative example, then some general statements follow.

4.1. Does the composition always worsen the TLS solvability? The following example illustrates that composition of core problems can counter-intuitively improve the TLS solvability class. First, we give a particular example of an $\mathcal{F}_1$ single right-hand side core problem. Then we start to compose it to obtain more complicated problems.

Example 4.1. Consider the approximation problem

$$\begin{bmatrix} a_l s \\ b_l c \end{bmatrix} x \approx \begin{bmatrix} a_l c \\ -b_l s \end{bmatrix}, \quad \text{where} \quad a_l > b_l > 0, \tag{4.1}$$
$$s = \sin(\varphi), \;\; c = \cos(\varphi), \;\; \varphi \neq \tfrac{1}{2}\pi k, \;\; k \in \mathbb{Z}.$$

Then

$$[B_1^{(l)}, A_{11}^{(l)}] \equiv \begin{bmatrix} a_l c & a_l s \\ -b_l s & b_l c \end{bmatrix} = I_2 \begin{bmatrix} a_l & 0 \\ 0 & b_l \end{bmatrix} \begin{bmatrix} c & -s \\ s & c \end{bmatrix}^{\mathrm{T}}$$

is in principle the SVD of the extended matrix. Since $m_l = 2$, $n_l = 1$, $d_l = 1$, so $\sigma_{n_l+1}^{(l)} = b_l$ is simple, so $q_l = 0$, $e_l = 1$, and $V_1^{(l)} = [c, s]$, $V_{12} = [s]$, and V_{13} has no columns. Consequently (4.1) is of class $\mathcal{F}_1$ and has a unique TLS solution.

To show that (4.1) is a core problem, we need to verify that it satisfies (CP1)–(CP3). Clearly $A_{11}^{(l)}$ as well as $B_1^{(l)}$ are of full column rank, i.e., (CP1) and (CP2) hold. Employing the SVD

$$A_{11}^{(l)} = \left(\frac{1}{\sqrt{(a_l s)^2 + (b_l c)^2}} \begin{bmatrix} a_l s & -b_l c \\ b_l c & a_l s \end{bmatrix} \right) \begin{bmatrix} \sqrt{(a_l s)^2 + (b_l c)^2} \\ 0 \end{bmatrix} [\,1\,]^{\mathrm{T}},$$

it is easy to see that both

$$\begin{aligned}(U_1')^{\mathrm{T}}B_1^{(l)} &= \left(\frac{1}{\sqrt{(a_l s)^2+(b_l c)^2}}\begin{bmatrix}a_l s\\ b_l c\end{bmatrix}\right)B_1^{(l)} = \frac{(a_l^2-b_l^2)cs}{\sqrt{(a_l s)^2+(b_l c)^2}},\\ (U_2')^{\mathrm{T}}B_1^{(l)} &= \left(\frac{1}{\sqrt{(a_l s)^2+(b_l c)^2}}\begin{bmatrix}-b_l c\\ a_l s\end{bmatrix}\right)B_1^{(l)} = \frac{-2a_l b_l}{\sqrt{(a_l s)^2+(b_l c)^2}}\end{aligned}$$

are (one-by-one) full row rank matrices, i.e., (CP3) is satisfied. Consequently (4.1) is a core problem of the class $\mathcal{F}_1$.

Now we take two particular choices of the parameters a_l, b_l in the example above, such that the composition of (4.1) with a single right-hand side degenerated component results in a core problem in $\mathcal{S}$ and $\mathcal{F}_1$, respectively.

Example 4.2. Consider the core problem (4.1) with $l=\alpha$, $a_\alpha=3$ and $b_\alpha=2$. Consider the core problem (4.1) with $l=\beta$, $a_\beta=5$, $b_\beta=1$. Compositions of these problems with the same degenerated component $[B_1^{(\gamma)}, A_{11}^{(\gamma)}]=[B_1^{(\gamma)}]=[4]$ (belonging also to $\mathcal{F}_1$), gives composed core problems with the following SVDs

$$\left[\begin{array}{cc|c}3c & 0 & 3s\\ -2s & 0 & 2c\\ 0 & 4 & 0\end{array}\right] = \begin{bmatrix}0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{bmatrix}\left[\begin{array}{c|c|c}4 & 0 & 0\\ 0 & 3 & 0\\ 0 & 0 & 2\end{array}\right]\left[\begin{array}{c|c|c}0 & c & -s\\ 1 & 0 & 0\\ \hline 0 & s & c\end{array}\right]^{\mathrm{T}}, \tag{4.2}$$

$$\left[\begin{array}{cc|c}5c & 0 & 5s\\ -1s & 0 & 1c\\ 0 & 4 & 0\end{array}\right] = \begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{bmatrix}\left[\begin{array}{c|c|c}5 & 0 & 0\\ 0 & 4 & 0\\ 0 & 0 & 1\end{array}\right]\left[\begin{array}{c|c|c}c & 0 & -s\\ 0 & 1 & 0\\ \hline s & 0 & c\end{array}\right]^{\mathrm{T}}, \tag{4.3}$$

respectively. The partitioning (2.3) of the matrices V is suggested by the lines. Then (4.2) is of class $\mathcal{S}$, while (4.3) remains in the class $\mathcal{F}_1$.

Thus we have two proper incompatible core problems (both with $d=2$) which we now compose together.

Example 4.3. Consider the core problems (4.2) and (4.3). Their composition results in a composed core problem with the following extended matrix and its SVD:

$$[B_1, A_{11}] = \left[\begin{array}{cccc|cc}B_1^{(\alpha)} & 0 & & & A_{11}^{(\alpha)} & \\ 0 & B_1^{(\gamma)} & & & 0 & \\ & & B_1^{(\beta)} & 0 & & A_{11}^{(\beta)}\\ & & 0 & B_1^{(\gamma)} & & 0\end{array}\right] = \left[\begin{array}{cccc|cc}3c & 0 & & & 3s & \\ -2s & 0 & & & 2c & \\ 0 & 4 & & & 0 & \\ & & 5c & 0 & & 5s\\ & & -1s & 0 & & 1c\\ & & 0 & 4 & & 0\end{array}\right]$$

$$= \begin{bmatrix} & & 0 & 1 & 0 & \\ & & 0 & 0 & 1 & \\ & & 1 & 0 & 0 & \\ 1 & 0 & & & & 0 \\ 0 & 0 & & & & 1 \\ 0 & 1 & & & & 0 \end{bmatrix} \left[\begin{array}{c|cc|ccc} 5 & 0 & & & & 0 \\ 0 & 4 & & & & 0 \\ & & 4 & 0 & 0 & \\ & & 0 & 3 & 0 & \\ & & 0 & 0 & 2 & \\ 0 & 0 & & & & 1 \end{array}\right] \left[\begin{array}{c|cc|ccc} & & 0 & c & -s & \\ & & 1 & 0 & 0 & \\ c & 0 & & & & -s \\ 0 & 1 & & & & 0 \\ \hline & & 0 & s & c & \\ s & 0 & & & & c \end{array}\right]^{\mathrm{T}}.$$

The partitioning (2.3) of V is again suggested by the lines. Clearly, we got a core problem with $d = 4$ that is of the class $\mathcal{F}_3$.

If we denote problems (4.2) and (4.3) as δ- and ε-component, respectively, the composition above can be schematically expressed as follows:

$$\underbrace{((\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma)}_{(\mathsf{CP}, 2, \mathcal{S})_\delta} \boxplus \underbrace{((\mathsf{CP}, 1, \mathcal{F}_1)_\beta \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma)}_{(\mathsf{CP}, 2, \mathcal{F}_1)_\varepsilon} = (\mathsf{CP}, 4, \mathcal{F}_3).$$

Now we look at the whole process the other way. Having in hand a problem of the class $\mathcal{S}$ (i.e., nongeneric one), its composition with a suitable $\mathcal{F}_1$ problem may result in a problem in $\mathcal{F}_3$ (i.e., it becomes generic). This can be seen as a form of *correction*, or *improvement* of the δ-component in terms of TLS solvability classes. Such improvement can be done in general, which will be investigated in the next section.

Remark 4.4. Since the core problems composition is associative and commutative (up to a permutation of components), the problem from Example 4.3 can also be expressed as follows (classes of the intermediate problems or components can be seen directly by crossing out suitable rows and columns of the SVD in Example 4.3):

$$\begin{aligned} (\mathsf{CP}, 4, \mathcal{F}_3) &= \underbrace{((\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta)}_{(\mathsf{CP}, 2, \mathcal{F}_1)_{\alpha \boxplus \beta}} \boxplus \underbrace{((\mathsf{CP}, 1, \mathcal{F}_1)_\gamma \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma)}_{(\mathsf{CP}, 2, \mathcal{F}_1)_{\gamma \boxplus \gamma}} \\ &= \underbrace{((\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma)}_{(\mathsf{CP}, 3, \mathcal{S})_{\alpha \boxplus \beta \boxplus \gamma}} \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma \\ &= \underbrace{((\mathsf{CP}, 1, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma)}_{(\mathsf{CP}, 3, \mathcal{F}_3)_{\alpha \boxplus \gamma \boxplus \gamma}} \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta \\ &= \underbrace{((\mathsf{CP}, 1, \mathcal{F}_1)_\beta \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\gamma)}_{(\mathsf{CP}, 3, \mathcal{F}_1)_{\beta \boxplus \gamma \boxplus \gamma}} \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\alpha. \end{aligned}$$

The first and the last row show that a composition of two $\mathcal{F}_1$ (in the first row one proper incompatible and one degenerated; in the last row two proper incompatible) components may result in an $\mathcal{F}_3$ problem. Recall that for two single right-hand side (i.e., $\mathcal{F}_1$) components, such composition is not possible (see Theorem 3.1 and the comment below), and therefore it was not observed in [2].

4.2. Improvement of nongeneric problems. The following theorem shows that it is always possible to move a nongeneric (i.e., class $\mathcal{S}$) core problem to the class of generic problems by composing it with another problem representing a sort of correction of the measured data, see Example 4.3.

Theorem 4.5. *Let* $A_{11}^{(\alpha)}X_{11}^{(\alpha)} \approx B_1^{(\alpha)}$, $A_{11}^{(\alpha)} \in \mathbb{R}^{m_\alpha \times n_\alpha}$, $B_1^{(\alpha)} \in \mathbb{R}^{m_\alpha \times d_\alpha}$ *be a core problem (that will serve as a component) and let it be in the class* $\mathcal{S}$. *Then there exists a component* $A_{11}^{(\beta)}X_{11}^{(\beta)} \approx B_1^{(\beta)}$, $A_{11}^{(\beta)} \in \mathbb{R}^{m_\beta \times n_\beta}$, $B_1^{(\beta)} \in \mathbb{R}^{m_\beta \times d_\beta}$ *such that the composed core problem*

$$A_{11}X_{11} \equiv \left(P^{\mathrm{T}} \begin{bmatrix} A_{11}^{(\alpha)} & 0 \\ 0 & A_{11}^{(\beta)} \end{bmatrix} Q\right) X_{11} \approx \left(P^{\mathrm{T}} \begin{bmatrix} B_1^{(\alpha)} & 0 \\ 0 & B_1^{(\beta)} \end{bmatrix} R\right) \equiv B_{11},$$

is in the class $\mathcal{F} = \mathcal{F}_1 \cup \mathcal{F}_2 \cup \mathcal{F}_3$.

Schematically: $\forall(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha$, $\exists(\mathsf{CP}, d_\beta, \mathcal{C})_\beta$ so that

$$(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{C})_\beta = (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{F}),$$

where $\mathcal{C} \in \{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{S}\}$ and $\mathcal{F} = \mathcal{F}_1 \cup \mathcal{F}_2 \cup \mathcal{F}_3$.

Proof. Let $[\,B_1^{(\alpha)}, A_{11}^{(\alpha)}\,] = U^{(\alpha)}\Sigma^{(\alpha)}(V^{(\alpha)})^{\mathrm{T}}$ be the SVD with the partitioning (2.3) of $V^{(\alpha)}$. Further, let

$$\sigma_1^{(\alpha)} \geqslant \sigma_2^{(\alpha)} \geqslant \ldots \geqslant \sigma_{n_\alpha - q_\alpha}^{(\alpha)},$$

be the singular values of $V_{11}^{(\alpha)}$. Let k be the number of distinct singular values of $V_{11}^{(\alpha)}$ with the multiplicities ϱ_j, $j = 1, \ldots, k$; i.e., $\sum_{j=1}^{k} \varrho_j = n_\alpha - q_\alpha$. Consider also a partitioning of $V_{11}^{(\alpha)}$ with respect to these multiplicities,

$$V_{11}^{(\alpha)} = [\,V_{11,1}^{(\alpha)}, V_{11,2}^{(\alpha)}, \ldots, V_{11,k}^{(\alpha)}\,] \in \mathbb{R}^{d_\alpha \times (n_\alpha - q_\alpha)}, \quad \text{with } V_{11,j}^{(\alpha)} \in \mathbb{R}^{d_\alpha \times \varrho_j}$$

being of full column ranks. Since the α-component is nongeneric, i.e., of class $\mathcal{S}$, $[V_{12}^{(\alpha)}, V_{13}^{(\alpha)}]$ has linearly dependent rows. Let t be defined so that

$$\begin{aligned} &\operatorname{rank}([\,V_{11,t}^{(\alpha)}, V_{11,t+1}^{(\alpha)}, \ldots, V_{11,k}^{(\alpha)}, V_{12}^{(\alpha)}, V_{13}^{(\alpha)}\,]) = d_\alpha, \quad \text{and} \\ &\operatorname{rank}([\,V_{11,t+1}^{(\alpha)}, \ldots, V_{11,k}^{(\alpha)}, V_{12}^{(\alpha)}, V_{13}^{(\alpha)}\,]) < d_\alpha. \end{aligned} \tag{4.4}$$

Now we construct a suitable β-component. Consider an arbitrary β-component such that it belongs to $\mathcal{F}_1$ (thus $[\,V_{12}^{(\beta)}, V_{13}^{(\beta)}\,] \in \mathbb{R}^{d_\beta \times d_\beta}$ is square invertible and $q_\beta = 0$) and

$$\sigma_{n_\beta+1}^{(\beta)} \equiv \sigma_{\varrho_1+\ldots+\varrho_{t-1}+1}^{(\alpha)} = \ldots = \sigma_{\varrho_1+\ldots+\varrho_{t-1}+\varrho_t}^{(\alpha)},$$

i.e., the e_β-tuple singular value of the β-component corresponding to $V_{12}^{(\beta)}$ is equal to the ϱ_t-tuple singular value of the α-component corresponding to $V_{11,t}^{(\alpha)}$. Then the block $V_1 \in \mathbb{R}^{d\times(n+d)}$ with $d = d_\alpha + d_\beta$, $n = n_\alpha + n_\beta$, from the SVD of the composed problem takes the form

$$V_1 = [V_{11}, V_{12}, V_{13}] = \left[\begin{array}{c|c|c} \begin{matrix} [V_{11,1}^{(\alpha)}, \ldots, V_{11,t-1}^{(\alpha)}] & 0 \\ 0 & V_{11}^{(\beta)} \end{matrix} & \underbrace{\begin{matrix} V_{11,t}^{(\alpha)} & 0 \\ 0 & V_{12}^{(\beta)} \end{matrix}}_{\varrho_t + e_\beta} & \underbrace{\begin{matrix} [V_{11,t+1}^{(\alpha)}, \ldots, V_{11,k}^{(\alpha)}], V_{12}^{(\alpha)}, V_{13}^{(\alpha)} & 0 \\ 0 & V_{13}^{(\beta)} \end{matrix}}_{(\varrho_{t+1}+\ldots+\varrho_k)+(d_\alpha+q_\alpha)+(d_\beta-e_\beta)} \end{array}\right] \left[\begin{array}{c|c|c} \Psi_{11} & & \\ \hline & I & \\ \hline & & \Psi_{13} \end{array}\right].$$

To align the blocks suggested by the vertical lines with the partitioning $[V_{11}, V_{12}, V_{13}]$, the $(n+1)$st (i.e., the dth last) column of V_1 has to be in $\begin{bmatrix} V_{11,t}^{(\alpha)} & 0 \\ 0 & V_{12}^{(\beta)} \end{bmatrix}$. Equivalently

$$d = d_\alpha + d_\beta > (\varrho_{t+1} + \ldots + \varrho_k) + (d_\alpha + q_\alpha) + (d_\beta - e_\beta), \quad \text{i.e.,}$$
$$e_\beta > (\varrho_{t+1} + \ldots + \varrho_k) + q_\alpha.$$

Recall that also $e_\beta \leqslant d_\beta$, see (2.2)–(2.3). Thus, put

$$e_\beta \equiv (\varrho_{t+1} + \ldots + \varrho_k) + q_\alpha + 1, \quad \text{and}$$
$$d_\beta \equiv (\varrho_{t+1} + \ldots + \varrho_k) + q_\alpha + 1 + \Delta, \quad \Delta \geqslant 0.$$

Then $V_{13}^{(\beta)} \in \mathbb{R}^{d_\beta \times \Delta}$ and $V_{13} \in \mathbb{R}^{(d_\alpha+d_\beta)\times((\varrho_{t+1}+\ldots+\varrho_k)+(d_\alpha+q_\alpha)+(d_\beta-e_\beta))} \equiv \mathbb{R}^{d\times(d-1)}$. We see that blocks are aligned and the $(n+1)$st (dth last) column of V_1 is exactly the last column of V_{12}. Since (4.4) is of full row rank d_α and $[\,V_{12}^{(\beta)}, V_{13}^{(\beta)}\,]$ is square invertible of rank d_β,

$$[V_{12}, V_{13}] = \left[\begin{array}{cc|cc} V_{11,t}^{(\alpha)} & 0 & [V_{11,t+1}^{(\alpha)}, \ldots, V_{11,k}^{(\alpha)}], V_{12}^{(\alpha)}, V_{13}^{(\alpha)} & 0 \\ 0 & V_{12}^{(\beta)} & 0 & V_{13}^{(\beta)} \end{array}\right] \left[\begin{array}{c|c} I & \\ \hline & \Psi_{13} \end{array}\right]$$

is also of full row rank $d = d_\alpha + d_\beta$, and thus the composed problem is of class $\mathcal{F}$.

It remains to show that there always exists a β-component satisfying all the requested properties. We take the simplest one,

$$(4.5) \qquad [B_1^{(\beta)}, A_{11}^{(\beta)}] = [B_1^{(\beta)}] \equiv \sigma_{\varrho_1+\ldots+\varrho_{t-1}+1}^{(\alpha)} I_{\varrho_{t+1}+\ldots+\varrho_k+q_\alpha+1},$$

i.e., $n_\beta = 0$ (it is a degenerated component), $m_\beta = d_\beta = e_\beta = (\varrho_{t+1}+\ldots+\varrho_k)+q_\alpha+1$, $\Delta = 0$, and $\sigma^{(\beta)}_{n_\beta+1} \equiv \sigma^{(\beta)}_1 = \sigma^{(\alpha)}_{\varrho_1+\ldots+\varrho_{t-1}+1}$ with the multiplicity e_β. The matrix $V^{(\beta)}$ from the SVD of $[B^{(\beta)}_1, A^{(\beta)}_{11}]$ contains only the block $V^{(\beta)}_{12}$ (the other blocks have no rows or columns, see (2.3) and the classification below). Moreover, $V^{(\beta)} = V^{(\beta)}_{12} = I_{\varrho_{t+1}+\ldots+\varrho_k+q_\alpha+1}$ is obviously square invertible. □

Note that we proved slightly stronger variant of Theorem 4.5. Instead of looking for a general β-component, we restricted ourselves first only to the class $\mathcal{F}_1$, and then only to the degenerated (class $\mathcal{F}_1$) components. However, such restriction was used only for simplicity and it is not necessary (see in particular Example 4.3).

Recall further the definition of t in (4.4). Instead of t, we may use any ϱ_τ and $V^{(\alpha)}_{11,\tau}$, $1 \leqslant \tau \leqslant t$, in the roles of ϱ_t and $V^{(\alpha)}_{11,t}$ for the construction of a β-component in the proof. In particular, we may simply use a degenerated β-component in the form[1] $[B^{(\beta)}_1, A^{(\beta)}_{11}] = [B^{(\beta)}_1] \equiv \sigma^{(\alpha)}_1 I_{n_\alpha+1}$ instead of (4.5). Our choice in (4.5) is in some sense the minimal one (since t is maximal among all τ's, $\Delta = 0$ is minimal among all Δ's, and both minimize the dimensions of the β-component).

Moreover, the resulting composed problem has in its SVD the block V_{13} that contains $\begin{bmatrix} V^{(\alpha)}_{12} & V^{(\alpha)}_{13} \\ 0 & 0 \end{bmatrix}$ as a submatrix. Since $[V^{(\alpha)}_{12}, V^{(\alpha)}_{13}] \in \mathbb{R}^{d_\alpha \times (d_\alpha+q_\alpha)}$, $q_\alpha \geqslant 0$, has linearly dependent rows and the number of its columns is larger than or equal to the number of columns, it has also linearly dependent columns. Thus also $\begin{bmatrix} V^{(\alpha)}_{12} & V^{(\alpha)}_{13} \\ 0 & 0 \end{bmatrix}$ and in particular V_{13} have linearly dependent columns. Consequently, the problem composed in the proof above does not belong to the classes $\mathcal{F}_1$ and $\mathcal{F}_2$. We actually proved that, schematically:

$\forall(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha$, $\exists$ $(\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta$ so that

$$(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{F}_3),$$

where the β-component is degenerated. This motivates a general result as follows.

Let us return back to the original, less restricted case: If we compose the α-component of the class $\mathcal{S}$ with an arbitrary β-component so that the resulting composed problem is in $\mathcal{F}$, then (see in particular (4.4)) $\begin{bmatrix} V^{(\alpha)}_{11,t} \\ 0 \end{bmatrix}$ and $\begin{bmatrix} V^{(\alpha)}_{12} & V^{(\alpha)}_{13} \\ 0 & 0 \end{bmatrix}$ have to be submatrices of $[V_{12}, V_{13}]$. Since the singular value corresponding to $V^{(\alpha)}_{11,t}$ is strictly larger than the singular value corresponding to $V^{(\alpha)}_{12}$, $\begin{bmatrix} V^{(\alpha)}_{12} & V^{(\alpha)}_{13} \\ 0 & 0 \end{bmatrix}$ is a submatrix of V_{13}. Consequently (as discussed above), if the composition results in an

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[1] Note that the so-called TLS algorithm when applied to the composed problem with this choice of a β-component returns a zero output.

$\mathcal{F}$ problem, it always belongs to $\mathcal{F}_3$. The classes $\mathcal{F}_1$ and $\mathcal{F}_2$ are not available. We formulate this observation as a corollary.

Corollary 4.6. *Let* $A^{(\alpha)}_{11} X^{(\alpha)}_{11} \approx B^{(\alpha)}_{1}$ *be a core problem in the class* $\mathcal{S}$*, and let* $A^{(\beta)}_{11} X^{(\beta)}_{11} \approx B^{(\beta)}_{1}$ *be an arbitrary core problem. Their composition cannot result in a problem in the class* $\mathcal{F}_1$ *or* $\mathcal{F}_2$*.*

Schematically: $\forall(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha$, $\forall(\mathsf{CP}, d_\beta, \mathcal{C})_\beta$,

$$(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{C})_\beta \neq (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{F}_1), (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{F}_2),$$

where $\mathcal{C} \in \{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{S}\}$.

In other words, we are able to *move a class* $\mathcal{S}$ *(nongeneric) problem to the class* $\mathcal{F}_3$ (generic, but without a TLS solution), but *no better result* is achievable by employing the approach above. The TLS solvability of a nongeneric core problem cannot be improved by its composition with another core problem.

4.3. Available and unavailable classes. Table 2 summarizes all the known available compositions of two core problems in terms of classes, see (2.7), Theorems 3.3, 3.2, Example 4.3, and Remark 4.4.

$\boxplus$	$\mathcal{F}_1$	$\mathcal{F}_2$	$\mathcal{F}_3$	$\mathcal{S}$
$\mathcal{F}_1$	$\mathcal{F}_1$, $\mathcal{F}_2$, $\mathcal{F}_3$, or $\mathcal{S}$ $\star$	sym.	sym.	sym.
$\mathcal{F}_2$	$\mathcal{F}_2$	$\mathcal{F}_2$	sym.	sym.
$\mathcal{F}_3$	$\mathcal{F}_3$		$\mathcal{F}_3$	sym.
$\mathcal{S}$	$\mathcal{F}_3$ or $\mathcal{S}$ $\star$			$\mathcal{S}$ $\star$

Table 2. List of *known available* compositions of two core problems (components) in terms of classes. Stars ($\star$) denote cases where all four possible results have been analyzed (cf. Table 3). The table is symmetric.

On the contrary, at the end of the previous section we have found for the first time a combination (of classes of components and a class of the resulting composed problem) that is not achievable. Consequently, it is clear that all 40 combinations are not available for core problem compositions. The following theorems discuss two more such cases. First we prove the assertion of Corollary 4.6 also for $\mathcal{F}_3$ problems. Then we show that a combination of two $\mathcal{S}$ class core problems results in a composed problem belonging again to $\mathcal{S}$.

Theorem 4.7. *Let* $A^{(\alpha)}_{11} X^{(\alpha)}_{11} \approx B^{(\alpha)}_{1}$ *be a core problem in the class* $\mathcal{F}_3$*, and let* $A^{(\beta)}_{11} X^{(\beta)}_{11} \approx B^{(\beta)}_{1}$ *be an arbitrary core problem. Their composition cannot result in a problem in the class* $\mathcal{F}_1$ *or* $\mathcal{F}_2$*.*

Schematically: $\forall(\mathsf{CP}, d_\alpha, \mathcal{F}_3)_\alpha$, $\forall(\mathsf{CP}, d_\beta, \mathcal{C})_\beta$,

$$(\mathsf{CP}, d_\alpha, \mathcal{F}_3)_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{C})_\beta \neq (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{F}_1),\ (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{F}_2),$$

where $\mathcal{C} \in \{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{S}\}$.

Proof. First of all note that the assertion is trivially true for $\mathcal{F}_3$ problems which are composed, and contain an $\mathcal{S}$ component (use Corollary 4.6 and the associativity of core problem composing). Now consider a general $\mathcal{F}_3$ problem as the α-component with partitioning of the matrix of right singular vectors as usual. Then the blocks of $V_1^{(\alpha)} = \big[V_{11}^{(\alpha)}, V_{12}^{(\alpha)}, V_{13}^{(\alpha)}\big] \in \mathbb{R}^{d_\alpha \times (n_\alpha + d_\alpha)}$ satisfy:

$$\begin{aligned} [V_{12}^{(\alpha)}, V_{13}^{(\alpha)}] \in \mathbb{R}^{d_\alpha \times (d_\alpha + q_\alpha)} &\quad \text{is of full row rank } d_\alpha \text{, and} \\ V_{13}^{(\alpha)} \in \mathbb{R}^{d_\alpha \times (d_\alpha - e_\alpha)} &\quad \text{has linearly dependent columns (and rows, } e_\alpha \geqslant 1\text{).} \end{aligned}$$

Recall that $V_{12}^{(\alpha)}$ corresponds to the singular value $\sigma_{n_\alpha+1}^{(\alpha)}$ with multiplicity $q_\alpha + e_\alpha$. Consider also the SVDs of the β-component and of the composed core problem, in particular the matrices $V_1^{(\beta)} \in \mathbb{R}^{d_\beta \times (n_\beta + d_\beta)}$ and $V_1 = [V_{11}, V_{12}, V_{13}] \in \mathbb{R}^{d \times (n+d)}$. Clearly,

$$V_1 = \begin{bmatrix} V_1^{(\alpha)} & 0 \\ 0 & V_1^{(\beta)} \end{bmatrix} \Psi = \begin{bmatrix} V_{11}^{(\alpha)} & V_{12}^{(\alpha)} & V_{13}^{(\alpha)} & 0 \\ 0 & 0 & 0 & V_1^{(\beta)} \end{bmatrix} \Psi,$$

where the permutation matrix Ψ sorts the singular values originated in both components into nonincreasing order. Thus Ψ does not change the ordering of columns of V_1 originated in one particular component, it only interlaces them with the columns originated in the other component.

Assume that the composed problem is in the class $\mathcal{F}$. Then $[V_{12}, V_{13}]$ is of full row rank. Since the α-component is of $\mathcal{F}_3$ and $V_{13}^{(\alpha)}$ has linearly dependent rows, $\begin{bmatrix} V_{12}^{(\alpha)} & V_{13}^{(\alpha)} \\ 0 & 0 \end{bmatrix}$ is a submatrix of $[V_{12}, V_{13}]$. Thus σ_{n+1} (the singular value corresponding to the V_{12} block of the composed problem) satisfies $\sigma_{n+1} \geqslant \sigma_{n_\alpha+1}$. Since $V_{13}^{(\alpha)}$ corresponds to singular values strictly smaller than σ_{n+1}, $\begin{bmatrix} V_{13}^{(\alpha)} \\ 0 \end{bmatrix}$ is a submatrix of V_{13}. Since $V_{13}^{(\alpha)}$ has linearly dependent columns, V_{13} has linearly dependent columns as well. Consequently, the composed problem cannot belong to $\mathcal{F}_1$ or $\mathcal{F}_2$. □

Theorem 4.5, Corollary 4.6, and Theorem 4.7 together are of particular importance. They show that while class $\mathcal{S}$ problems can be moved to $\mathcal{F}_3$ (but no better improvement is possible), $\mathcal{F}_3$ problems cannot be improved further. Consequently, *the set of $\mathcal{F}_3$ and $\mathcal{S}$ core problems is in some sense closed with respect to compositions with core problems from other classes.* This indicates that the distinction between $\mathcal{F}_3$ and $\mathcal{S}$ problems is rather artificial, as it originated in the generic—nongeneric classification introduced in [10]. Recall that in both $\mathcal{F}_3$ and $\mathcal{S}$, the TLS solution does not exist. Now we show that the class $\mathcal{S}$ is closed in a slightly weaker sense.

Theorem 4.8. *Composition of two (or more) class $\mathcal{S}$ core problems always results in a class $\mathcal{S}$ problem.*

Schematically: $\forall(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha$, $\forall(\mathsf{CP}, d_\beta, \mathcal{S})_\beta$,

$$(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{S})_\beta = (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{S}),$$

or equivalently

$$(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{S})_\beta \neq (\mathsf{CP}, d_\alpha + d_\beta, \mathcal{F}), \quad \mathcal{F} = \mathcal{F}_1 \cup \mathcal{F}_2 \cup \mathcal{F}_3.$$

Proof. Let $A_{11}^{(l)} X_{11}^{(l)} \approx B_1^{(l)}$, $A_{11}^{(l)} \in \mathbb{R}^{m_l \times n_l}$, $B_1^{(l)} \in \mathbb{R}^{m_l \times d_l}$ for $l = \alpha, \beta$ be two core problems in the class $\mathcal{S}$. Consider their SVDs $[B_1^{(l)}, A_{11}^{(l)}] = U^{(l)} \Sigma^{(l)} (V^{(l)})^{\mathrm{T}}$, with the partitionings

$$V^{(l)} = \begin{bmatrix} V_1^{(l)} \\ V_2^{(l)} \end{bmatrix} = \begin{bmatrix} V_{11}^{(l)} & V_{12}^{(l)} & V_{13}^{(l)} \\ V_{21}^{(l)} & V_{22}^{(l)} & V_{23}^{(l)} \end{bmatrix} \begin{matrix} \}\, d_l \\ \}\, n_l \end{matrix} \qquad \operatorname{rank}([\, V_{12}^{(l)}, V_{13}^{(l)}\,]) < d_l.$$

We are interested in the singular values $\sigma_{n_l+1}^{(l)}$, $l = \alpha, \beta$. There are two cases: Either $\sigma_{n_\alpha+1}^{(\alpha)} = \sigma_{n_\beta+1}^{(\beta)}$, or $\sigma_{n_\alpha+1}^{(\alpha)} > \sigma_{n_\beta+1}^{(\beta)}$ (the third case $\sigma_{n_\alpha+1}^{(\alpha)} < \sigma_{n_\beta+1}^{(\beta)}$ is essentially the same as the second, only with the exchanged roles of α- and β-components).

Case 1. Let $\sigma_{n_\alpha+1}^{(\alpha)} = \sigma_{n_\beta+1}^{(\beta)}$. Then the SVD of

$$[B_1, A_{11}] = P^{\mathrm{T}} \left[\begin{array}{cc|cc} B_1^{(\alpha)} & 0 & A_{11}^{(\alpha)} & 0 \\ 0 & B_1^{(\beta)} & 0 & A_{11}^{(\beta)} \end{array}\right] \left[\begin{array}{c|c} R & 0 \\ \hline 0 & Q \end{array}\right]$$

gives V with the structure

$$V_1 = R^{\mathrm{T}} \left[\begin{array}{cc|cc|cc} V_{11}^{(\alpha)} & 0 & V_{12}^{(\alpha)} & 0 & V_{13}^{(\alpha)} & 0 \\ 0 & V_{11}^{(\beta)} & 0 & V_{12}^{(\beta)} & 0 & V_{13}^{(\beta)} \end{array}\right] \left[\begin{array}{c|c|c} \Psi_{11} & & \\ \hline & I & \\ \hline & & \Psi_{13} \end{array}\right] \in \mathbb{R}^{d \times (n+d)},$$

where $n \equiv n_\alpha + n_\beta$, $d \equiv d_\alpha + d_\beta$. It remains to verify whether the vertical lines correspond to the partitioning of $V_1 = [V_{11}, V_{12}, V_{13}]$ with respect to σ_{n+1}, i.e., whether σ_{n+1} is the singular value $\sigma_{n_\alpha+1}^{(\alpha)} = \sigma_{n_\beta+1}^{(\beta)}$.

Since $V_{11}^{(l)} \in \mathbb{R}^{d_l \times (n_l - q_l)}$, we have $\begin{bmatrix} V_{11}^{(\alpha)} & 0 \\ 0 & V_{11}^{(\beta)} \end{bmatrix} \in \mathbb{R}^{d \times (n - q_\alpha - q_\beta)}$. Because $q_l \geqslant 0$, we have $n - q_\alpha - q_\beta < n + 1$, i.e., the $(n+1)$th column of V_1 does not belong to the first block. Similarly, from $V_{13}^{(l)} \in \mathbb{R}^{d_l \times (d_l - e_l)}$ we get $\begin{bmatrix} V_{13}^{(\alpha)} & 0 \\ 0 & V_{13}^{(\beta)} \end{bmatrix} \in \mathbb{R}^{d \times (d - e_\alpha - e_\beta)}$. Because $e_l \geqslant 1$, then $d > d - e_\alpha - e_\beta$, i.e., the $(n+1)$th column (which is actually also the dth last column of V_1) does not belong to this last block.

Consequently, $\sigma_{n+1} = \sigma_{n_\alpha+1}^{(\alpha)} = \sigma_{n_\beta+1}^{(\beta)}$ and it has multiplicity $q + e$, where $q \equiv q_\alpha + q_\beta$ is its left-, and $e \equiv e_\alpha + e_\beta$ is its right-multiplicity. Since both $[V_{12}^{(l)}, V_{13}^{(l)}]$ for $l = \alpha, \beta$, have linearly dependent rows, $[V_{11}, V_{12}]$ has linearly dependent rows as well, i.e., $\operatorname{rank}([V_{11}, V_{12}]) < d$. Finally, the composed problem is of the class $\mathcal{S}$.

Case 2. Let $\sigma_{n_\alpha+1}^{(\alpha)} > \sigma_{n_\beta+1}^{(\beta)}$. Then the SVD of the extended matrix gives V with much more complicated structure of V_1. Here the relations between $\sigma_1^{(\beta)}, \ldots, \sigma_{n_\beta}^{(\beta)}$ and $\sigma_{n_\alpha+1}^{(\alpha)}$ have to be taken into account. In particular there may be singular values strictly larger than, equal to, and smaller than $\sigma_{n_\alpha+1}^{(\alpha)}$. To reflect this, we introduce the formal partitioning

$$V_{11}^{(\beta)} = [V_{11\mathsf{A}}^{(\beta)}, V_{11\mathsf{B}}^{(\beta)}, V_{11\mathsf{C}}^{(\beta)}] \in \mathbb{R}^{d_\beta \times (n_\beta - q_\beta)}$$

without specifying the dimensions of the individual blocks. Then

$$V_1 = R^{\mathrm{T}} \left[\begin{array}{cc|cc|cccc} V_{11}^{(\alpha)} & 0 & V_{12}^{(\alpha)} & 0 & V_{13}^{(\alpha)} & 0 & 0 & 0 \\ 0 & V_{11\mathsf{A}}^{(\beta)} & 0 & V_{11\mathsf{B}}^{(\beta)} & 0 & V_{11\mathsf{C}}^{(\beta)} & V_{12}^{(\beta)} & V_{13}^{(\beta)} \end{array}\right] \left[\begin{array}{c|c|c} \Psi_{11} & & \\ \hline & I & \\ \hline & & \Psi_{13} \end{array}\right],$$

but the partitioning suggested by the vertical lines *may not* correspond to the partitioning of $V_1 = [V_{11}, V_{12}, V_{13}]$ with respect to σ_{n+1}. However, the number of columns of the first suggested block is less than, or equal to $n - q_\alpha - q_\beta$. Since $q_l \geqslant 0$, we have $n - q_\alpha - q_\beta < n + 1$ and thus the $(n+1)$st column of V_1 is either in the second, or in the third of the suggested blocks. The matrix $[V_{12}, V_{13}]$ is then in general a *submatrix* of the matrix formed by the last two suggested blocks.

Since $[V_{12}^{(\alpha)}, V_{13}^{(\alpha)}]$ has linearly dependent rows, the matrix formed by the last two suggested blocks has linearly dependent rows, i.e., it is of the rank strictly smaller than d. Therefore, any of its submatrices is of rank strictly smaller than d, and in particular $\operatorname{rank}([V_{11}, V_{12}]) < d$. Thus the composed problem is of class $\mathcal{S}$. $\square$

Table 2 of known available compositions of core problems (in terms of classes) can now be complemented by a list of known unavailable compositions in Table 3, see Corrolary 4.6 and Theorem 4.8. Both tables together indicate combinations that require further investigation.

$\boxplus$	$\mathcal{F}_1$	$\mathcal{F}_2$	$\mathcal{F}_3$	$\mathcal{S}$
$\mathcal{F}_1$	— *	sym.	sym.	sym.
$\mathcal{F}_2$			sym.	sym.
$\mathcal{F}_3$	$\mathcal{F}_1$ and $\mathcal{F}_2$	$\mathcal{F}_1$ and $\mathcal{F}_2$	$\mathcal{F}_1$ and $\mathcal{F}_2$	sym.
$\mathcal{S}$	$\mathcal{F}_1$ and $\mathcal{F}_2$ *	$\mathcal{F}_1$ and $\mathcal{F}_2$	$\mathcal{F}_1$ and $\mathcal{F}_2$	$\mathcal{F}_1$, $\mathcal{F}_2$, and $\mathcal{F}_3$ *

Table 3. List of *known unavailable* compositions of two core problems (components) in terms of classes. Stars ($\star$) denote cases where all four possible results have been analyzed (cf. Table 2). The table is symmetric.

5. EXISTENCE OF IRREDUCIBLE CORE PROBLEMS IN VARIOUS CLASSES

All particular examples of core problems discussed in the previous sections (e.g., when filling up Table 2) have been composed from single right-hand side components. However, in [2] it was shown that there exists an irreducible (nondecomposable) core problem with $d = 2$ in $\mathcal{F}_2$. For completeness, we show by examples that there exist irreducible core problems with $d = 2$ also in $\mathcal{F}_1$ and $\mathcal{S}$. Recall that an $\mathcal{F}_3$ problem with $d = 2$ does not exist, see Table 1.

Example 5.1. Consider three problems $A_{11}X_1 \approx B_1$, $A_{11} \in \mathbb{R}^{4\times 2}$, $B_1 \in \mathbb{R}^{4\times 2}$ given in forms of SVDs of their extended matrices:

$$[B_1, A_{11}] = I_4 \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \left(\frac{1}{3} \left[\begin{array}{cc|c|c} -1 & -3 & \sqrt{3} & \sqrt{3} \\ 3 & -1 & \sqrt{3} & -\sqrt{3} \\ \hline \sqrt{3} & \sqrt{3} & 1 & 3 \\ \sqrt{3} & -\sqrt{3} & -3 & 1 \end{array}\right] \right)^{\mathrm{T}}, \tag{5.1}$$

$$[B_1, A_{11}] = I_4 \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \left(\frac{1}{3} \left[\begin{array}{c|cc|c} -1 & -3 & \sqrt{3} & \sqrt{3} \\ 3 & -1 & \sqrt{3} & -\sqrt{3} \\ \hline \sqrt{3} & \sqrt{3} & 1 & 3 \\ \sqrt{3} & -\sqrt{3} & -3 & 1 \end{array}\right] \right)^{\mathrm{T}}, \tag{5.2}$$

$$[B_1, A_{11}] = I_4 \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \left(\frac{1}{2} \left[\begin{array}{cc|c|c} \sqrt{2} & \sqrt{2} & 0 & 0 \\ -1 & 1 & -1 & 1 \\ \hline 0 & 0 & \sqrt{2} & \sqrt{2} \\ 1 & -1 & -1 & 1 \end{array}\right] \right)^{\mathrm{T}}. \tag{5.3}$$

The second problem has already been presented in [3] and [2], it is included for completeness. Note that the matrix of the left singular vectors may be chosen arbitrarily, we use I_4 for simplicity. The partitioning of the right-most matrices of the right singular vectors corresponds to (2.3). Clearly, the problems above belong to the class $\mathcal{F}_1$, $\mathcal{F}_2$, and $\mathcal{S}$, respectively.

Now we show that they represent core problems. Since all three matrices $[B_1, A_{11}]$ are of full column rank, A_{11} and B_1 are also of full column rank. Thus the problems satisfy (CP1) and (CP2). Matrices A_{11} have simple singular values

$$\varsigma_{1,2} = \frac{1}{2}\sqrt{25 \pm 3\sqrt{2}}, \quad \varsigma_{1,2} = \sqrt{4 \pm \frac{3\sqrt{5}}{8}}, \quad \varsigma_{1,2} = \sqrt{5 \pm \frac{\sqrt{2}\sqrt{59}}{4}},$$

respectively. It is easy to find their left and right singular vectors (e.g., by using MATLAB with Symbolic Math Toolbox)[2], and to verify that (CP3) is satisfied as well. Consequently, all problems represent core problems with the SVD forms

$$\left[\begin{array}{cc|cc} b_{11} & b_{12} & \varsigma_1 & 0 \\ b_{21} & b_{22} & 0 & \varsigma_2 \\ b_{31} & b_{32} & 0 & 0 \\ b_{41} & b_{42} & 0 & 0 \end{array}\right], \quad \varsigma_1 > \varsigma_2 > 0, \tag{5.4}$$

where the only two free parameters (up to sign changes) are hidden in:

▷ the transformation of the right-hand side $B_1 = \widetilde{B}_1 G_R^{\mathrm{T}}$ by some orthogonal matrix $G_R^{\mathrm{T}} = G_R^{-1} \in \mathbb{R}^{2\times 2}$; and

▷ the choice of the orthonormal basis (let it be stored in the columns of the matrix U_3') of the two-dimensional $\mathcal{N}(A_{11}^{\mathrm{T}})$, i.e., $U_3' = \widetilde{U}_3' G_L^{\mathrm{T}}$, $G_L^{\mathrm{T}} = G_L^{-1} \in \mathbb{R}^{2\times 2}$.

Both of them involve the left bottom block of (5.4), in particular

$$\begin{bmatrix} b_{31} & b_{32} \\ b_{41} & b_{42} \end{bmatrix} = (U_3')^{\mathrm{T}} B_1 = G_L((\widetilde{U}_3')^{\mathrm{T}} \widetilde{B}_1) G_R^{\mathrm{T}}. \tag{5.5}$$

It remains to show that the problems are irreducible. In general, if a core problem is composed, its SVD form must be composable from SVD forms of its individual components. Recalling that any single right-hand side component in the SVD form has the right-hand side with all entries being nonzero (see [8]), the right-hand side of a composed core problem in the SVD form (5.4) must be orthogonally transformable to a chess-board-like pattern of zero and (strictly) nonzero blocks. Consequently, if $[B_1, A_{11}]$ is composed then there exist orthogonal matrices (elementary Givens rotations) G_L and G_R transforming (5.5) to a chess-board structured $(\widetilde{U}_3')^{\mathrm{T}} \widetilde{B}_1$. Since (5.5) is of full row rank (see (CP3)), the only possibility is to (anti)diagonalize it. But with diagonal $(\widetilde{U}_3')^{\mathrm{T}} \widetilde{B}_1$, (5.5) in principle represents an SVD of $\begin{bmatrix} b_{31} & b_{32} \\ b_{41} & b_{42} \end{bmatrix}$

---

[2] See for example the code included as supplementary material to [2]. MATLAB codes for verification (by numerical and symbolic calculation) for all three problems are on request freely available by the authors.

Calculation of this SVD therefore fixes the free parameters represented by G_L, G_R. Application of these matrices to the whole (5.4) then either reveals the chess-board structure, if the problem is composed, or not, if it is irreducible. Now it is easy to verify that neither of the three problem is composed.

There is no systematic method for the construction of irreducible core problems with the given number of right-hand sides in the given class. However, the examples above support the expectation that there exist irreducible core problems in all classes for any $d \geqslant 3$.

6. Conclusions

In this paper, we have investigated solvability classes of core problems within linear approximation problems with multiple observations. We have presented the full solvability classification revealing that, in particular, the core problem with two right-hand sides cannot be in the class $\mathcal{F}_3$. Then we have concentrated on the relations between solvability classes while core problems composing. It has been shown that any nongeneric (class $\mathcal{S}$) problem can be moved to generic (class $\mathcal{F}_3$) by employing a particular data correction represented by a composition with a single right-hand side core problem. However, the TLS solution of the corrected problem still does not exist. We have shown that the set of core problems without a TLS solution (i.e., $\mathcal{F}_3 \cup \mathcal{S}$) is closed with respect to composing its elements with components from other classes. Moreover, the set of core problems in the class $\mathcal{S}$ is closed with respect to composing its elements together. Finally, we have presented examples of irreducible core problems with two right-hand sides in all available classes.

The main results are summarized in Tables 1, 2, and 3. Results can be divided into four types of assertions ($\mathcal{C} \in \{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, \mathcal{S}\}$):

Existential (based on examples)
$\exists(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha$, $\exists(\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta$: $(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha{+}d_\beta, \mathcal{F}_1)$.
$\exists(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha$, $\exists(\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta$: $(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha{+}d_\beta, \mathcal{F}_2)$.
$\exists(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha$, $\exists(\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta$: $(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha{+}d_\beta, \mathcal{F}_3)$.
$\exists(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha$, $\exists(\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta$: $(\mathsf{CP}, d_\alpha, \mathcal{F}_1)_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha{+}d_\beta, \mathcal{S})$.

Semi-general
$\forall(\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha$, $\exists(\mathsf{CP}, 1, \mathcal{F}_1)_\beta$: $(\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha \boxplus (\mathsf{CP}, 1, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha{+}1, \mathcal{C})$.
$\forall(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha$, $\exists(\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta$: $(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{F}_1)_\beta = (\mathsf{CP}, d_\alpha{+}d_\beta, \mathcal{F}_3)$.

General (positive)
$\forall(\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha$: $(\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha \boxplus (\mathsf{CP}, d_\alpha, \mathcal{C})_\alpha = (\mathsf{CP}, 2d_\alpha, \mathcal{C})$.
$\forall(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha$, $\forall(\mathsf{CP}, d_\beta, \mathcal{S})_\beta$: $(\mathsf{CP}, d_\alpha, \mathcal{S})_\alpha \boxplus (\mathsf{CP}, d_\beta, \mathcal{S})_\beta = (\mathsf{CP}, d_\alpha{+}d_\beta, \mathcal{S})$.

General (negative)
$\forall(\mathsf{CP},1,\mathcal{F}_1)_\alpha$, $\forall(\mathsf{CP},1,\mathcal{F}_1)_\beta$: $(\mathsf{CP},1,\mathcal{F}_1)_\alpha \boxplus (\mathsf{CP},1,\mathcal{F}_1)_\beta \neq (\mathsf{CP},2,\mathcal{F}_3)$.
$\forall(\mathsf{CP},d_\alpha,\mathcal{F}_3)_\alpha$, $\forall(\mathsf{CP},d_\beta,\mathcal{C})_\beta$: $(\mathsf{CP},d_\alpha,\mathcal{S})_\alpha \boxplus (\mathsf{CP},d_\beta,\mathcal{C})_\beta \neq (\mathsf{CP},d_\alpha{+}d_\beta,\mathcal{F}_1)$.
$\forall(\mathsf{CP},d_\alpha,\mathcal{F}_3)_\alpha$, $\forall(\mathsf{CP},d_\beta,\mathcal{C})_\beta$: $(\mathsf{CP},d_\alpha,\mathcal{S})_\alpha \boxplus (\mathsf{CP},d_\beta,\mathcal{C})_\beta \neq (\mathsf{CP},d_\alpha{+}d_\beta,\mathcal{F}_2)$.
$\forall(\mathsf{CP},d_\alpha,\mathcal{S})_\alpha$, $\forall(\mathsf{CP},d_\beta,\mathcal{C})_\beta$: $(\mathsf{CP},d_\alpha,\mathcal{S})_\alpha \boxplus (\mathsf{CP},d_\beta,\mathcal{C})_\beta \neq (\mathsf{CP},d_\alpha{+}d_\beta,\mathcal{F}_1)$.
$\forall(\mathsf{CP},d_\alpha,\mathcal{S})_\alpha$, $\forall(\mathsf{CP},d_\beta,\mathcal{C})_\beta$: $(\mathsf{CP},d_\alpha,\mathcal{S})_\alpha \boxplus (\mathsf{CP},d_\beta,\mathcal{C})_\beta \neq (\mathsf{CP},d_\alpha{+}d_\beta,\mathcal{F}_2)$.

We see that the TLS solvability of a core problem is strongly influenced by composing, and till now, it is not clear how to detect the possible (ir)reducibility in general. Therefore, understanding the properties of the composed problems is important for the analysis and solution of TLS problems in general.

Acknowledgements. We wish to thank the anonymous referee for her or his careful reading the paper and useful comments which led to improvements of our manuscript.

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PART III

CORE REDUCTION FOR PROBLEMS IN GENERALIZED SETTINGS

6 POSSIBLE WAYS OF MATRIX RIGHT-HAND SIDE PROBLEM GENERALIZATION

In this part we present several ways of possible generalizations of matrix right-hand side linear approximation problems as we have already outlined in Chapter 2 and sketched in Figure 2.2. The directions of generalization (or specialization when looking from bottom to top) can be seen in the following scheme

$$\begin{tikzcd}
& Ax \approx b \arrow[d] & & \text{where} \quad A \in \mathbb{R}^{m\times n},\ x \in \mathbb{R}^{n},\ b \in \mathbb{R}^{m} \\
& AX \approx B \arrow[dl] \arrow[dr] & & \text{where} \quad A \in \mathbb{R}^{m\times n},\ X \in \mathbb{R}^{n\times d},\ B \in \mathbb{R}^{m\times d} \\
A \times_1 \mathcal{X} \approx \mathcal{B}, \arrow[dr] & & A_{\mathsf{L}} X A_{\mathsf{R}}^{\mathsf{T}} \approx B \arrow[dl] & \begin{cases} A \in \mathbb{R}^{m\times n},\ \mathcal{X} \in \mathbb{R}^{n\times d_2\times\cdots\times d_k},\ \mathcal{B} \in \mathbb{R}^{m\times d_2\times\cdots\times d_k} \\ A_{\mathsf{L}} \in \mathbb{R}^{m\times n},\ A_{\mathsf{R}} \in \mathbb{R}^{d\times c},\ X \in \mathbb{R}^{n\times c},\ B \in \mathbb{R}^{m\times d} \end{cases} \\
& (A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) \approx \mathcal{B}, & & \text{where} \quad \begin{cases} A_s \in \mathbb{R}^{m_s\times n_s}, \quad \text{for } s = 1, 2, \ldots, k, \\ \mathcal{X} \in \mathbb{R}^{n_1\times n_2\times\cdots\times n_k},\ \mathcal{B} \in \mathbb{R}^{m_1\times m_2\times\cdots\times m_k}. \end{cases}
\end{tikzcd}$$

Namely, the problem with tensor right-hand side (third line left) is covered in Chapter 7, the bilinear problem with matrix right-hand side (third line right) is covered in Chapter 8, and the most general multilinear (or k-linear) problem with tensor right-hand side (fourth line) is covered in Chapter 9.

Note here that when working with tensors we use the notation established in [14] and [15]. The above (in the third line) mentioned product $A_s \times_s \mathcal{X}$ of the matrix $A_s = (a_{i,j}) \in \mathbb{R}^{m_s\times n_s}$ and the tensor $\mathcal{X} = (x_{i_1,i_2,\ldots,i_k}) \in \mathbb{R}^{n_1\times n_2\times\cdots\times n_k}$ in sth mode is defined as

$$(A_s \times_s \mathcal{X})_{i_1,\ldots,i_{s-1},i,i_{s+1},\ldots,i_k} = \sum\nolimits_{\ell=1}^{n_s} a_{i,\ell} \cdot x_{i_1,\ldots,i_{s-1},\ell,i_{s+1},\ldots,i_k} .$$

Then the other product (in the fourth line) of a tensor with more matrices of suitable dimensions is defined analogously, and denoted

$$(A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) = A_1 \times_1 (A_2 \times_2 (\cdots \times_{k-1} (A_k \times_k \mathcal{X}) \cdots)).$$

Each of Chapters 7–9 introduces the particular linear approximation problem including the formulation of TLS minimization, then introduces the core problem within, and the way how it was derived. We also point out important properties of core problems and note on available results on solvability. The results on this topic have already been published in a series of papers, whose copies are included in the end of this part.

7 PROBLEM WITH TENSOR RIGHT-HAND SIDE

The most straightforward way to generalize problems with vector and matrix right-hand sides is by adding dimension. This means that there will be a tensor on the right hand-side and therefore also a solution of the problem will be a tensor. Such problems arise in various applications such as 3D imaging problems, time-dependent 2D problems, or models arising from linearization of problems depending on several parameters; see for example [23], [20], [24]. Results connected to this topic are published in [8]; see also the copy enclosed on page 141.

7.1 PROBLEM FORMULATION AND THE TLS MINIMIZATION

First, we formulate the problem. By linear approximation problem with tensor right-hand side we mean

$$A \times_1 \mathcal{X} \approx \mathcal{B}, \qquad A \in \mathbb{R}^{m \times n},\ \mathcal{X} \in \mathbb{R}^{n \times d_2 \times \cdots \times d_k},\ \mathcal{B} \in \mathbb{R}^{m \times d_2 \times \ldots \times d_k}; \tag{7.1}$$

see [8]. By solving such problem in the TLS sense we mean, analogously to previous simpler cases (see Chapter 1), solving the minimization problem

$$\min_{\substack{\mathcal{G} \in \mathbb{R}^{m \times d_2 \times \cdots \times d_k} \\ E \in \mathbb{R}^{m \times n}}} \left(\|\mathcal{G}\|^2 + \|E\|_F^2 \right)^{\frac{1}{2}} \tag{7.2}$$

$$\text{subject to} \qquad \exists\, \mathcal{X}_{\mathsf{TLS}} \in \mathbb{R}^{n \times d_2 \times \cdots \times d_k} \ :\ (A + E) \times_1 \mathcal{X}_{\mathsf{TLS}} = \mathcal{B} + \mathcal{G}.$$

We call it the TLS problem with tensor right-hand side. Note that we use the tensor norm as it is defined in [15], i.e.,

$$\|\mathcal{G}\| \equiv \left(\sum_{i_1=1}^{m} \sum_{i_2=1}^{d_2} \cdots \sum_{i_k=1}^{d_k} g_{i_1, i_2, \ldots, i_k}^2 \right)^{\frac{1}{2}},$$

which is a straightforward generalization of the 2-norm of a vector, or Frobenius norm of a matrix.

Remark 3 (on TLS solvability)**.** *Let us define the matricization of a tensor* $\mathcal{T} \in \mathbb{R}^{t_1 \times \cdots \times t_k}$ *in mode* s *— simply the matrix* $\mathcal{T}^{\{s\}} \in \mathbb{R}^{t_s \times (\Delta_{\mathcal{T}}/t_s)}$*, where* $\Delta_{\mathcal{T}} \equiv \prod_{\ell=1}^{k} t_\ell$*, containing the* s*-mode fibres (the generalization of the concept of rows and columns) of tensor* $\mathcal{T}$*, as columns, in the inverse lexicographical order w.r.t. their multi-indices; see [15]. Then, in particular*

$$(A_s \times_s \mathcal{X})^{\{s\}} = A_s \, \mathcal{X}^{\{s\}}, \qquad \text{and} \qquad \|\mathcal{G}\| = \|\mathcal{G}^{\{s\}}\|_F;$$

see [15]. Consequently, TLS minimization (7.2) can be fully re-formulated in matrix fashion. Moreover, (7.2) is equivalent to

$$\min_{\substack{\mathcal{G} \in \mathbb{R}^{m \times d_2 \times \cdots \times d_k} \\ E \in \mathbb{R}^{m \times n}}} \left(\|\mathcal{G}\|^2 + \|E\|_F^2 \right)^{\frac{1}{2}} \quad \text{subject to} \quad \mathcal{R}\Big((\mathcal{B} + \mathcal{G})^{\{1\}} \Big) \subseteq \mathcal{R}(A + E);$$

or even to

$$\min_{\substack{G \in \mathbb{R}^{m \times (\Delta_{\mathcal{B}}/m)} \\ E \in \mathbb{R}^{m \times n}}} \big\| [\begin{array}{cc} G & E \end{array}] \big\|_F \quad \text{subject to} \quad \mathcal{R}\Big(\mathcal{B}^{\{1\}} + G \Big) \subseteq \mathcal{R}(A + E);$$

see also [8]. Note that the last one is the very standard matrix right-hand side TLS formulation (1.7). This allows to switch between the tensor and the fully matricized formulations. Therefore, all the results on TLS solvability and the whole TLS solvability analysis can be directly adopted from the matrix to the tensor right-hand side case.

7.2 CORE PROBLEM WITHIN $A \times_1 \mathcal{X} \approx \mathcal{B}$

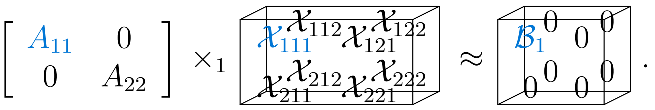
Since the TLS minimization (7.2) for the tensor right-hand side problem (7.1) uses orthogonally invariant norms, we can apply an orthogonal transformation realized by $(k+1)$ orthogonal matrices

$$(P, Q, R_2, \ldots, R_k) \in \mathbb{O}_m \times \mathbb{O}_n \times \mathbb{O}_{d_2} \times \cdots \times \mathbb{O}_{d_k},$$

so the minimization in (7.2) stays unchanged. This transformation leads to the modified problem

$$(P^{\mathsf{T}} A Q) \times_1 (Q^{\mathsf{T}}, R_2^{\mathsf{T}}, \ldots, R_k^{\mathsf{T}} \,|\, \mathcal{X}) \approx (P^{\mathsf{T}}, R_2^{\mathsf{T}}, \ldots, R_k^{\mathsf{T}} \,|\, \mathcal{B}). \tag{7.3}$$

The goal is to find such an orthogonal transformation that the modified problem has a block diagonal structure (tensors illustrated as being of order three for clarity)



(7.4)

The original problem is, therefore, partitioned into 2^k subproblems, in particular,

$$A_{11} \times_1 \mathcal{X}_{11\ldots1} \approx \mathcal{B}_1, \qquad A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}},\ \mathcal{X}_{11\ldots1} \in \mathbb{R}^{\overline{n}\times\overline{d}_2\times\cdots\times\overline{d}_k},\ \mathcal{B}_1 \in \mathbb{R}^{\overline{m}\times\overline{d}_2\times\ldots\times\overline{d}_k},$$

and

$$\begin{aligned} A_{11} \times_1 \mathcal{X}_{1i_2\ldots i_k} &\approx 0, \qquad (i_2,\ldots,i_k) \in \Big(\{1,2\}^{k-1} \setminus (1,\ldots,1)\Big), \\ A_{22} \times_1 \mathcal{X}_{2j_2\ldots j_k} &\approx 0, \qquad (j_2,\ldots,j_k) \in \{1,2\}^{k-1}. \end{aligned}$$

The only subproblem we need to solve is the first one; the others obviously have zero solutions. The first subproblem with minimal dimensions (among all possible orthogonal transformations yielding this block structure) is called the core problem; see [8].

7.3 CORE PROBLEM REDUCTION FOR $A \times_1 \mathcal{X} \approx \mathcal{B}$

The core problem reduction within the problem with the tensor right-hand side was published in [8] (notation in the paper differs from the notation here; we prefer simplicity in the paper, whereas consistency among individual reductions here). It generalizes the procedure of the core problem reduction for matrix right-hand side problems; see [6]. In the following text we summarize four basic steps of the reduction:

- Right-hand side preprocessing (Section 7.3.1).
- Transformation of the system matrix (Section 7.3.2).
- Partitioning and transformation of the right-hand side (Section 7.3.3).
- Final permutation (Section 7.3.5).

The reduction uses the SVD of the system matrix A and the Tucker decomposition (or HOSVD standing for the high-order SVD, which is a generalization of SVD for tensors) of the tensor of the right-hand side $\mathcal{B}$; see [25], [26], [27]; we also refer to [15], where is a great review of the arithmetics of tensors and tensor decompositions. The Tucker decomposition of the right-hand side tensor $\mathcal{B} \in \mathbb{R}^{m\times d_2\times\cdots\times d_k}$ takes full and economical forms

$$\begin{aligned} \mathcal{B} &= \big(\, R_1, R_2, \ldots, R_k \,\big|\, \mathsf{diag}_k(\mathcal{B}_{\mathsf{TC}}, 0_{m-r_1,d_2-r_2,\ldots,d_k-r_k}) \,\big) \\ &= \big(\, R_1', R_2', \ldots, R_k' \,\big|\, \mathcal{B}_{\mathsf{TC}} \,\big). \end{aligned} \tag{7.5}$$

Here

$$r_s = \mathsf{rank}(\mathcal{B}^{\{s\}}), \qquad s = 1, 2, \ldots, k,$$

are ranks of individual s-mode matricizations. Matrices

$$R_1 = [R_1', R_1''] \in \mathbb{O}_m, \quad R_1' \in \mathbb{R}^{m\times r_1},$$

and $\qquad R_s = [R_s', R_s''] \in \mathbb{O}_{d_s}, \quad R_s' \in \mathbb{R}^{d_s\times r_s}, \qquad s = 2,\ldots,k;$

moreover, all R_s (i.e., $s = 1, 2, \dots, k$) are square orthogonal matrices of left singular vectors from the SVDs of $\mathcal{B}^{\{s\}}$ and R'_s contain only vectors corresponding to nonzero singular values. Finally, $\mathcal{B}_{\mathsf{TC}}$ is the so-called Tucker core, and diag_k realizes the block diagonal composition of the given two tensors of order k along the k-dimensional diagonal. (Note that the term Tucker core is not related to the core problem terminology.)

7.3.1 Preprocessing of a right-hand side

In the first step we use matrices R_s and R'_s from the Tucker decomposition of tensor $\mathcal{B}$ (7.5) in order to transform the original problem (7.1) to

$$A \times_1 \left(I_n, R_2^{\mathsf{T}}, \dots, R_k^{\mathsf{T}} \,\middle|\, \mathcal{X} \right) \equiv \left(A, R_2^{\mathsf{T}}, \dots, R_k^{\mathsf{T}} \,\middle|\, \mathcal{X} \right) \approx \left(I_m, R_2^{\mathsf{T}}, \dots, R_k^{\mathsf{T}} \,\middle|\, \mathcal{B} \right). \quad (7.6)$$

This allows us to split the original problem to 2^{k-1} subproblems. Only the first subproblem has nonzero right-hand side — the Tucker core — and thus needs to be solved, i.e.,

$$A \times_1 \mathcal{X}' \approx \mathcal{B}', \quad (7.7)$$

where

$$\mathcal{B}' \equiv \left(I_m, R_2'^{\mathsf{T}}, \dots, R_k'^{\mathsf{T}} \,\middle|\, \mathcal{B} \right) = \left(R'_1, I_{r_2}, \dots, I_{r_k} \,\middle|\, \mathcal{B}_{\mathsf{TC}} \right) \in \mathbb{R}^{m \times r_2 \times \cdots \times r_k} \quad \text{and}$$
$$\mathcal{X}' \equiv \left(I_n, R_2'^{\mathsf{T}}, \dots, R_k'^{\mathsf{T}} \,\middle|\, \mathcal{X} \right) \in \mathbb{R}^{n \times r_2 \times \cdots \times r_k}.$$

The remaining $(2^{k-1} - 1)$ problems have zero right-hand sides and therefore also zero solutions. Matrices $\mathcal{B}'^{\{s\}}$, i.e., s-mode matricizations of the right-hand side tensor $\mathcal{B}'$ are of *full row rank equal to r_s having mutually orthogonal rows* for all $s = 2, \dots, k$, thanks to the Tucker decomposition.

7.3.2 Transformation of the system matrix

In the next step we aim to transform the system matrix to a simpler (diagonal) form. We use the SVD of the matrix A, i.e.,

$$A = U \Sigma V^{\mathsf{T}}, \qquad U \in \mathbb{O}_m, \quad \Sigma \in \mathbb{R}^{m \times n}, \quad V \in \mathbb{O}_n.$$

Let A have ξ distinct nonzero singular values

$$\sigma_1 > \sigma_2 > \cdots > \sigma_\xi > 0,$$

and let μ_i, $i = 1, \dots, \xi$, be their multiplicities, i.e.,

$$\sum_{i=1}^{\xi} \mu_i = \mathrm{rank}(A).$$

Further, denote

$$\mu_{\xi+1} \equiv m - \mathrm{rank}(A) = \dim(\mathcal{N}(A^{\mathsf{T}})), \quad \nu_{\xi+1} \equiv n - \mathrm{rank}(A) = \dim(\mathcal{N}(A)).$$

Thus

$$\Sigma = \text{diag}\big(\, \sigma_1 I_{\mu_1}\, ,\ \dots\ ,\ \sigma_\xi I_{\mu_\xi}\, ,\ 0_{\mu_{\xi+1},\nu_{\xi+1}}\big). \tag{7.8}$$

The SVD is then used to transform problem (7.7) so that

$$\begin{gathered}(U^\mathsf{T} A V) \times_1 (V^\mathsf{T} \times_1 \mathcal{X}') \approx (U^\mathsf{T} \times_1 \mathcal{B}'),\\ \Sigma \times_1 \mathcal{Y} \approx \mathcal{F},\end{gathered} \tag{7.9}$$

with diagonal system matrix, and where

$$\begin{aligned}\mathcal{Y} &= V^\mathsf{T} \times_1 \mathcal{X}' = \big(\, V^\mathsf{T}, I_{r_2}, \dots, I_{r_k} \,\big|\, \mathcal{X}' \,\big) = \big(\, V^\mathsf{T}, R_2'^\mathsf{T}, \dots, R_k'^\mathsf{T} \,\big|\, \mathcal{X} \,\big) \in \mathbb{R}^{n \times r_2 \times \cdots \times r_k},\\ \mathcal{F} &= U^\mathsf{T} \times_1 \mathcal{B}' = \big(\, U^\mathsf{T}, I_{r_2}, \dots, I_{r_k} \,\big|\, \mathcal{B}' \,\big) = \big(\, U^\mathsf{T}, R_2'^\mathsf{T}, \dots, R_k'^\mathsf{T} \,\big|\, \mathcal{B} \,\big) \in \mathbb{R}^{m \times r_2 \times \cdots \times r_k}.\end{aligned}$$

7.3.3 Partitioning and transformation of the right-hand side

In the next step we will transform the right-hand side while preserving the already achieved diagonal structure of the system matrix. The goal of this transformation is to get as many zero blocks (in the form of whole zero fibres) in the right-hand side tensor as possible. In order to do that, we consider the following partitioning of $\mathcal{F}$ w.r.t. multiplicities of singular values of A, i.e.,

$$\mathcal{F}^{\{1\}} = \begin{bmatrix} F_1 \\ \vdots \\ F_\xi \\ F_{\xi+1} \end{bmatrix} \in \mathbb{R}^{m \times (\Delta_\mathcal{F}/m)}, \qquad \text{where} \qquad F_i \in \mathbb{R}^{\mu_i \times (\Delta_\mathcal{F}/m)},$$

for $i = 1, \dots, \xi, \xi+1$, and where $\Delta_\mathcal{F} = m \cdot \prod_{\ell=2}^{k} r_\ell$. Recall that all the other matricizations of tensor $\mathcal{F}$, i.e.,

$$\mathcal{F}^{\{s\}} \in \mathbb{R}^{r_s \times (\Delta_\mathcal{F}/r_s)}, \qquad s = 2, \dots, k,$$

are of *full row rank equal to* r_s *having mutually orthogonal rows* (due to the right-hand side preprocessing). Let

$$\overline{\mu}_i = \text{rank}(F_i)$$

and consider (semi-economical) SVDs

$$F_i = L_i \begin{bmatrix} \Theta_i \\ 0_{\mu_i - \overline{\mu}_i, \overline{\mu}_i} \end{bmatrix} W_i'^\mathsf{T},$$

where

$$L_i \in \mathbb{O}_{\mu_i}, \quad \Theta_i \in \mathbb{R}^{\overline{\mu}_i \times \overline{\mu}_i}, \quad W_i' \in \mathbb{R}^{(\Delta_\mathcal{F}/m) \times \overline{\mu}_i},$$

and where, in particular:

- Θ_i is diagonal invertible of order $\overline{\mu}_i$, and
- W_i' have orthonormal columns, i.e., $W_i'^\mathsf{T} W_i' = I_{\overline{\mu}_i}$,

for $i = 1, \ldots, \xi, \xi + 1$.

Define orthogonal matrices

$$L_U \equiv \text{diag}(L_1, \ldots, L_\xi, L_{\xi+1}) \in \mathbb{O}_m,$$
$$L_V \equiv \text{diag}(L_1, \ldots, L_\xi, I_{\nu_{\xi+1}}) \in \mathbb{O}_n,$$

Since (7.8), we get

$$L_U^\mathsf{T} \Sigma L_V = \Sigma,$$

so the problem (7.9) can be further transformed, while preserving diagonal system matrices, to

$$\begin{gathered} (L_U^\mathsf{T} \Sigma L_V) \times_1 (L_V^\mathsf{T} \times_1 \mathcal{Y}) \approx (L_U^\mathsf{T} \times_1 \mathcal{F}), \\ \Sigma \times_1 \mathcal{Z} \approx \mathcal{H}, \end{gathered} \tag{7.10}$$

with diagonal system matrix, and where

$$\begin{aligned} \mathcal{Z} &= L_V^\mathsf{T} \times_1 \mathcal{Y} = \left(L_V^\mathsf{T}, I_{r_2}, \ldots, I_{r_k} \,\middle|\, \mathcal{Y} \right) \in \mathbb{R}^{n \times r_2 \times \cdots \times r_k}, \qquad \text{and} \\ \mathcal{H} &= L_U^\mathsf{T} \times_1 \mathcal{F} = \left(L_U^\mathsf{T}, I_{r_2}, \ldots, I_{r_k} \,\middle|\, \mathcal{F} \right) \in \mathbb{R}^{m \times r_2 \times \cdots \times r_k}. \end{aligned}$$

7.3.4 Note on structure of the right-hand side

It would be useful to look at the structure of the new right-hand side of (7.10). Clearly,

$$\mathcal{H}^{\{1\}} = (L_U^\mathsf{T} \times_1 \mathcal{F})^{\{1\}} = L_U^\mathsf{T} \mathcal{F}^{\{1\}} = \begin{bmatrix} L_1^\mathsf{T} F_1 \\ \vdots \\ L_\xi^\mathsf{T} F_\xi \\ L_{\xi+1}^\mathsf{T} F_{\xi+1} \end{bmatrix} \in \mathbb{R}^{m \times (\Delta_\mathcal{H}/m)}$$

has block-rows

$$L_i^\mathsf{T} F_i = \begin{bmatrix} \Theta_i W_i'^\mathsf{T} \\ 0_{\mu_i - \overline{\mu}_i, \Delta_\mathcal{F}/m} \end{bmatrix} \equiv \begin{bmatrix} H_i \\ 0_{\mu_i - \overline{\mu}_i, \Delta_\mathcal{F}/m} \end{bmatrix} \in \mathbb{R}^{\mu_i \times (\Delta_\mathcal{H}/m)},$$

with $\overline{\mu}_i$ nonzero and mutually orthogonal rows (followed by $\mu_i - \overline{\mu}_i$ zero rows). Consequently, since the full row rank matrix

$$H_i \in \mathbb{R}^{\overline{\mu}_i \times (\Delta_\mathcal{H}/m)}$$

is a block-row in 1-mode matricization of tensor $\mathcal{H}$, this tensor contains blocks

$$\mathcal{H}_i \in \mathbb{R}^{\overline{\mu}_i \times r_2 \times \cdots \times r_k}, \qquad \text{such that} \qquad \mathcal{H}_i^{\{1\}} = H_i,$$

followed by zero blocks $0_{\mu_i - \overline{\mu}_i, r_2, \ldots, r_k}$, for $i = 1, \ldots, \xi, \xi + 1$.

7.3.5 Final permutation

Now we want to aggregate the relevant information revealed in the nonzero blocks of the right-hand side $\mathcal{H}$ to get the block structure as in (7.4). To achieve that we need to find permutation moving the nonzero block $\mathcal{H}_i$, i.e., nonzero block-rows H_i of $\mathcal{H}^{\{1\}}$ up while moving the zero block-rows down. It can be realized by the permutation matrix

$$\Pi_U \equiv \left[\begin{array}{cccc|cccc} \left[\begin{smallmatrix} I_{\overline{\mu}_1} \\ 0 \end{smallmatrix}\right] & & 0 & 0 & \left[\begin{smallmatrix} 0 \\ I_{\mu_1-\overline{\mu}_1} \end{smallmatrix}\right] & & 0 & 0 \\ & \ddots & & \vdots & & \ddots & & \vdots \\ 0 & & \left[\begin{smallmatrix} I_{\overline{\mu}_\xi} \\ 0 \end{smallmatrix}\right] & 0 & 0 & & \left[\begin{smallmatrix} 0 \\ I_{\mu_\xi-\overline{\mu}_\xi} \end{smallmatrix}\right] & 0 \\ 0 & \cdots & 0 & \left[\begin{smallmatrix} I_{\overline{\mu}_{\xi+1}} \\ 0 \end{smallmatrix}\right] & 0 & \cdots & 0 & \left[\begin{smallmatrix} 0 \\ I_{\mu_{\xi+1}-\overline{\mu}_{\xi+1}} \end{smallmatrix}\right] \end{array}\right] \in \mathbb{O}_m,$$

since

$$\begin{aligned} (\Pi_U^{\mathsf{T}} \times_1 \mathcal{H})^{\{1\}} &= \Pi_U^{\mathsf{T}} \mathcal{H}^{\{1\}} \\ &= \Pi_U^{\mathsf{T}} \left[\begin{array}{c} \left[\begin{array}{c} H_1 \\ 0_{\mu_1-\overline{\mu}_1,\Delta_{\mathcal{H}}/m} \end{array}\right] \\ \vdots \\ \left[\begin{array}{c} H_\xi \\ 0_{\mu_\xi-\overline{\mu}_\xi,\Delta_{\mathcal{H}}/m} \end{array}\right] \\ \left[\begin{array}{c} H_{\xi+1} \\ 0_{\mu_{\xi+1}-\overline{\mu}_{\xi+1},\Delta_{\mathcal{H}}/m} \end{array}\right] \end{array}\right] = \left[\begin{array}{c} H_1 \\ \vdots \\ H_\xi \\ H_{\xi+1} \\ \hline 0_{m-\overline{m},\Delta_{\mathcal{H}}/m} \end{array}\right] \equiv \left[\begin{array}{c} \mathcal{B}_1^{\{1\}} \\ 0_{m-\overline{m},\Delta_{\mathcal{H}}/m} \end{array}\right], \end{aligned}$$

where $\overline{m} = \sum_{i=1}^{\xi+1} \overline{\mu}_i$. We see that we interpret the upper nonzero part of the tensor $(\Pi_U^{\mathsf{T}} \times_1 \mathcal{H})$ as

$$\mathcal{B}_1 \in \mathbb{R}^{\overline{m} \times r_2 \times \cdots \times r_k},$$

i.e., the core problem right-hand side tensor; see (7.4).

The multiplication of the whole approximation problem $\Sigma \times_1 \mathcal{Z} \approx \mathcal{H}$ by the permutation matrix Π_U^{T} in the first mode, i.e., the application of Π_U^{T} from the left on its 1-mode matricization $\Sigma \mathcal{Z}^{\{1\}} \approx \mathcal{H}^{\{1\}}$,

$$(\Pi_U^{\mathsf{T}} \times_1 (\Sigma \times_1 \mathcal{Z}))^{\{1\}} = \Pi_U^{\mathsf{T}} (\Sigma \times_1 \mathcal{Z})^{\{1\}} = \Pi_U^{\mathsf{T}} (\Sigma \mathcal{Z}^{\{1\}}) = (\Pi_U^{\mathsf{T}} \Sigma) \mathcal{Z}^{\{1\}} \approx \Pi_U^{\mathsf{T}} \mathcal{H}^{\{1\}},$$

results in shuffling the diagonal structure of the system matrix Σ. In order to keep the system matrices as much diagonal as possible — in particular block-diagonal with diagonal blocks — we need another permutation matrix that compensates the action of the first permutation as much as possible. It is easy to see that such matrix is

$$\Pi_V \equiv \left[\begin{array}{ccc|cccc} \left[\begin{smallmatrix} I_{\overline{\mu}_1} \\ 0 \end{smallmatrix}\right] & & 0 & \left[\begin{smallmatrix} 0 \\ I_{\mu_1-\overline{\mu}_1} \end{smallmatrix}\right] & & 0 & 0 \\ & \ddots & & & \ddots & & \vdots \\ 0 & & \left[\begin{smallmatrix} I_{\overline{\mu}_\xi} \\ 0 \end{smallmatrix}\right] & 0 & & \left[\begin{smallmatrix} 0 \\ I_{\mu_\xi-\overline{\mu}_\xi} \end{smallmatrix}\right] & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & I_{\nu_{\xi+1}} \end{array}\right] \in \mathbb{O}_n.$$

Then

$$\begin{aligned}\Pi_U^{\mathsf{T}}\,\Sigma\,\Pi_V = \mathrm{diag}\Big(& \overbrace{\mathrm{diag}(\sigma_1 I_{\overline{\mu}_1}, \ldots, \sigma_\xi I_{\overline{\mu}_\xi}, 0_{\overline{\mu}_{\xi+1},0})}^{A_{11}}, \\ & \underbrace{\mathrm{diag}(\sigma_1 I_{\mu_1-\overline{\mu}_1}, \ldots, \sigma_\xi I_{\mu_\xi-\overline{\mu}_\xi}, 0_{\mu_{\xi+1}-\overline{\mu}_{\xi+1},\nu_{\xi+1}})}_{A_{22}}\Big) \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix}\end{aligned} \tag{7.11}$$

is the wanted block-diagonal structure; see (7.4).

7.3.6 Summary of the reduction

Let us summarize the whole reduction. Starting with (7.1) we proceed: right-hand side preprocessing (7.7), transformation based on SVD of the system matrix (7.9), right-hand side decomposition (7.10), and final permutation. In total we get

$$\begin{aligned}\Big((\Pi_U^{\mathsf{T}} L_U^{\mathsf{T}} U^{\mathsf{T}})\, A\, (V L_V \Pi_V) \Big) \times_1 \Big((\Pi_V^{\mathsf{T}} L_V^{\mathsf{T}} V^{\mathsf{T}}), R_2^{\mathsf{T}}, \ldots, R_k^{\mathsf{T}} \,\big|\, \mathcal{X} \Big) & \\ \approx \Big((\Pi_U^{\mathsf{T}} L_U^{\mathsf{T}} U^{\mathsf{T}}), R_2^{\mathsf{T}}, \ldots, R_k^{\mathsf{T}} \,\big|\, \mathcal{B} \Big)&,\end{aligned}$$

i.e.,

$$\begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \times_1 \widetilde{\mathcal{X}} \approx \mathrm{diag}_k(\mathcal{B}_1, 0_{m-\overline{m}, d_2-\overline{d}_2, \ldots, d_k-\overline{d}_k}),$$

the core problem revealing transformation (7.3), (7.4). Clearly,

$$P = U L_U \Pi_U, \quad \text{and} \quad Q = V L_V \Pi_V,$$

and

$$\overline{m} = \sum_{i=1}^{\xi+1} \overline{\mu}_i, \quad \overline{n} = \sum_{i=1}^{\xi} \overline{\mu}_i, \quad \text{and} \quad \overline{d}_s = r_s, \quad \text{for} \quad s = 1, \ldots, k.$$

The minimality of this construction is discussed in [8]; see also [6].

Remark 4. *Note that the matrices $R_s = [R_s', R_s'']$ originated in the right-hand side preprocessing stay unchanged during the rest of the whole process. However, till this moment we worked only with their parts R_s'; now we use the whole orthogonal matrices. It was only in order simplify the exposition. Using the parts causes the reduction of the right-hand side tensor while omitting all the zero 1-mode fibres; these are, however, not influenced by the first orthogonal matrix. Now we want to describe the whole orthogonal transformation.*

7.4 PROPERTIES OF CORE PROBLEM WITHIN $A \times_1 \mathcal{X} \approx \mathcal{B}$

The above described core problem reduction guarantees the following properties of the core problem

$$A_{11} \times_1 \mathcal{X}_{11\ldots1} \approx \mathcal{B}_1$$

within the linear approximation problem with tensor right-hand side (see [8]):

$*$(CP1) $A_{11} \in \mathbb{R}^{\overline{m} \times \overline{n}}$ is of *full column rank* equal to $\overline{n}$.
$*$(CP2) $\mathcal{B}_1^{\{s\}} \in \mathbb{R}^{\overline{d}_s \times (\Delta_{\mathcal{B}_1}/\overline{d}_s)}$ are of *full row rank* equal to $\overline{d}_s$, for $s = 2, \ldots, k$.
$*$(CP3) $U_i^{\mathsf{T}} \mathcal{B}_1^{\{1\}} \in \mathbb{R}^{\overline{\mu}_i \times (\Delta_{\mathcal{B}_1}/\overline{m})}$ are of *full row rank* equal to $\overline{\mu}_i$, for $i = 1, \ldots, \overline{\xi}, \overline{\xi} + 1$.
(CP4) $[\mathcal{B}_1^{\{1\}}, A_{11}] \in \mathbb{R}^{\overline{m} \times (\overline{n} + \Delta_{\mathcal{B}_1}/\overline{m})}$ is of *full row rank* equal to $\overline{m}$.

Recall that we denote $\Delta_{\mathcal{B}_1} = \overline{m} \cdot \prod_{\ell=2}^{k} \overline{d}_\ell$, and columns of U_i form the basis of the ith left singular vector subspaces of A_{11} (including the null-space of A_{11}^{T}). Among the above listed properties of the core problem, the first three asterisked are in fact equivalent to the minimality of such subproblem. Note that the core problem has a bunch of further interesting properties; see in particular [8] and also [11, Appendix A].

Remark 5 (on TLS solvability). *Here we are in a very specific situation — the TLS minimization for the tensor right-hand side problem is equivalent to the TLS minimization of its matricized version; see Remark 3. Thus, we may consider core problem reductions of both, the tensor problem and its matricized counterpart, schematically:*

$$\begin{tikzcd}
A \times_1 \mathcal{X} \approx \mathcal{B} \arrow[r, "\text{CPR}"] \arrow[d, leftrightarrow, "\text{(de)matricization}"'] & A_{11} \times_1 \mathcal{X}_{11\cdots1} \approx \mathcal{B}_1 \\
AX \approx \mathcal{B}^{\{1\}} \equiv B \arrow[r, "\text{CPR}"] & A_{11} X_1 \approx B_1
\end{tikzcd}$$

Obviously, we can try to close the loop in this diagram and to consider two matrix right-hand side problems:

- *the matricized & then reduced* $[B_1, A_{11}]$,
- *and the reduced & then matricized* $[\mathcal{B}_1^{\{1\}}, A_{11}]$,

and the straightforward question will be, whether both are the same.

First, from properties (CP1) and (CP3) of the matrix and of the tensor right-hand side problems we easily get that both problems share the same system matrix A_{11} *(up to possible orthogonal transformation). However, the right-hand sides are in general different. The reason is simple: the core problem reduction in the tensor settings needs to keep the tensor structure* *of the right-hand side. In particular, it cannot reduce all the 1-mode fibres of $\mathcal{B}$ to the linearly independent set of size $\overline{d}$, because the total number of remaining fibres needs to be the product of $(k-1)$ (rather general) natural numbers $\overline{d}_\ell$, i.e., in general*

$$\overline{d} \leq \prod_{\ell=2}^{k} \overline{d}_\ell.$$

Compare (CP2) properties for both core problems (we reformulate the first one using transposition):

(CP2) $B_1^\mathsf{T} \in \mathbb{R}^{\overline{d}\times\overline{m}}$ *is of full row rank equal to* $\overline{d}$.

(CP2) $\mathcal{B}_1^{\{s\}} \in \mathbb{R}^{\overline{d}_s\times(\Delta_{\mathcal{B}_1}/\overline{d}_s)}$ *are of full row rank equal to* $\overline{d}_s$*, for* $s = 2, \ldots, k$.

Comparing both transformations (1.11) and (7.3) we can immediately see that both right-hand sides are the same (up to an orthogonal transformation) when

$$R = R_k \otimes \cdots \otimes R_2,$$

i.e., when the matrix R from the standard matrix core problem reduction has this special so-called Kronecker product (denoted by $\otimes$) structure.

Consequently, in terms of ordering (see Chapters 4 and 5),

$$B_1 \sqsubseteq \mathcal{B}_1^{\{1\}}, \qquad \text{and} \qquad \begin{bmatrix} B_1 & A_{11} \end{bmatrix} \sqsubseteq \begin{bmatrix} \mathcal{B}_1^{\{1\}} & A_{11} \end{bmatrix}.$$

In other words, the tensor core problem $A_{11} \times_1 \mathcal{X}_{11\cdots1} \approx \mathcal{B}_1$ can be further reduced after matricization in general. Since the true (final) matrix core problem $A_{11}X_1 \approx B_1$ may belong to any of the TLS solvability classes $\mathcal{F}_1$, $\mathcal{F}_2$, $\mathcal{F}_3$, and $\mathcal{S}$ (see [5], [4], and [10]), we presume the same behaviour of the tensor right-hand side core problem in general.

8 BILINEAR PROBLEM WITH MATRIX RIGHT-HAND SIDE

In some real applications problems with bilinear models naturally arise (see [16] and [17] for the problem formulation and their application). Results connected to this topic are published in [9]; see the copy enclosed on page 167.

8.1 PROBLEM FORMULATION AND THE TLS MINIMIZATION

Let us introduce the approximation problem with a bilinear model and matrix right-hand side

$$A_{\mathsf{L}} X A_{\mathsf{R}}^{\mathsf{T}} \approx B, \qquad A_{\mathsf{L}} \in \mathbb{R}^{m\times n},\ A_{\mathsf{R}} \in \mathbb{R}^{d\times c},\ X \in \mathbb{R}^{n\times c},\ B \in \mathbb{R}^{m\times d}; \tag{8.1}$$

see [9]. The TLS minimization can be generalized as follows

$$\min_{\substack{G \in \mathbb{R}^{m\times d} \\ E_{\mathsf{L}} \in \mathbb{R}^{m\times n} \\ E_{\mathsf{R}} \in \mathbb{R}^{d\times c}}} \left\| \begin{bmatrix} G & E_{\mathsf{L}} \\ E_{\mathsf{R}}^{\mathsf{T}} & 0 \end{bmatrix} \right\|_F \tag{8.2}$$

$$\text{subject to} \qquad \exists\, X_{\mathsf{TLS}} \in \mathbb{R}^{n\times c} \ :\ (A_{\mathsf{L}} + E_{\mathsf{L}})\, X_{\mathsf{TLS}}\, (A_{\mathsf{R}} + E_{\mathsf{R}})^{\mathsf{T}} = (B + G),$$

see [9]. We call it the bilinear TLS problem with matrix right-hand side.

Remark 6 (on TLS solvability). *In this case, even though there are no tensors in the game and it is fully matrix formulated, the TLS solvability analysis for the matrix right-hand side problems as presented in [5] cannot be simply used. Some analogy or generalization of solvability classes $\mathcal{F}_1$, $\mathcal{F}_2$, $\mathcal{F}_3$, and $\mathcal{S}$, has not been studied yet (up to the knowledge of the author).*

On the other hand, some results in this direction (however discussed from the more practical computational point of view) are already presented in the works [16] and [17].

8.2 CORE PROBLEM WITHIN $A_L X A_R^{\mathsf{T}} \approx B$

Making use of the orthogonal invariance of the norm in the TLS minimization (8.2), we can transform the problem (8.1) with four orthogonal matrices

$$(P, Q, R, K) \in \mathbb{O}_m \times \mathbb{O}_n \times \mathbb{O}_c \times \mathbb{O}_d$$

such that

$$(P^{\mathsf{T}} A_{\mathsf{L}} Q)\,(Q^{\mathsf{T}} X R)\,(R^{\mathsf{T}} A_{\mathsf{R}}^{\mathsf{T}} K) \approx (P^{\mathsf{T}} B K), \tag{8.3}$$

and the minimization in (8.2) stays unchanged.

The goal is to find such orthogonal transformation yielding a block diagonal structure of the problem

$$\begin{bmatrix} A_{\mathsf{L},11} & 0 \\ 0 & A_{\mathsf{L},22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} A_{\mathsf{R},11} & 0 \\ 0 & A_{\mathsf{R},22} \end{bmatrix}^{\mathsf{T}} \approx \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{8.4}$$

The original problem can be, therefore, partitioned into four subproblems, in particular,

$$A_{\mathsf{L},11} X_{11} A_{\mathsf{R},11}^{\mathsf{T}} \approx B_1, \qquad A_{\mathsf{L},11} \in \mathbb{R}^{\overline{m} \times \overline{n}},\ A_{\mathsf{R},11} \in \mathbb{R}^{\overline{d} \times \overline{c}},\ X_{11} \in \mathbb{R}^{\overline{n} \times \overline{c}},\ B_1 \in \mathbb{R}^{\overline{m} \times \overline{d}},$$

and

$$A_{\mathsf{L},11} X_{12} A_{\mathsf{R},22}^{\mathsf{T}} \approx 0, \qquad A_{\mathsf{L},22} X_{22} A_{\mathsf{R},22}^{\mathsf{T}} \approx 0, \qquad A_{\mathsf{L},22} X_{21} A_{\mathsf{R},11}^{\mathsf{T}} \approx 0.$$

The only subproblem we need to solve is the first one; the other three obviously have zero solutions. The first subproblem with minimal dimensions (among all possible orthogonal transformations yielding this block structure) is called the core problem; see [9].

8.3 CORE PROBLEM REDUCTION FOR $A_L X A_R^{\mathsf{T}} \approx B$

The core problem reduction within the bilinear problem with the matrix right-hand side was published in [9] (notation in the paper differs from the notation here; we prefer simplicity in the paper, whereas consistency among individual reductions here). It generalizes the procedure of the core problem reduction for matrix right-hand side problems; see [6]. The procedure now consists of only three steps:

- Transformation of the system matrices (Section 8.3.1).
- Partitioning and transformation of the right-hand side (Section 8.3.2).
- Final permutation (Section 8.3.4).

The right-hand side preprocessing is not necessary here, it is done implicitly.

8.3.1 Transformation of the system matrices

First, we want to transform the matrices A_{L} and A_{R} to the diagonal forms. Therefore, we start with their SVDs, i.e.,

$$\begin{aligned} A_{\mathsf{L}} &= U_{\mathsf{L}}\Sigma V_{\mathsf{L}}^{\mathsf{T}}, &\quad U_{\mathsf{L}} &\in \mathbb{O}_m, &\quad \Sigma &\in \mathbb{R}^{m\times n}, &\quad V_{\mathsf{L}} &\in \mathbb{O}_n, \\ A_{\mathsf{R}} &= U_{\mathsf{R}}\Psi V_{\mathsf{R}}^{\mathsf{T}}, & U_{\mathsf{R}} &\in \mathbb{O}_d, & \Psi &\in \mathbb{R}^{d\times c}, & V_{\mathsf{R}} &\in \mathbb{O}_c. \end{aligned}$$

Let A_{L} and A_{R} have ξ and ζ *distinct* nonzero singular values, respectively,

$$\sigma_1 > \sigma_2 > \cdots > \sigma_\xi > 0, \qquad \text{and} \qquad \psi_1 > \psi_2 > \cdots > \psi_\zeta > 0,$$

and let μ_i, $i = 1, \ldots, \xi$, and δ_j, $j = 1, \ldots, \zeta$, be their multiplicities, respectively, i.e.,

$$\sum_{i=1}^{\xi} \mu_i = \mathsf{rank}(A_{\mathsf{L}}), \qquad \text{and} \qquad \sum_{j=1}^{\zeta} \delta_j = \mathsf{rank}(A_{\mathsf{R}}).$$

Further, denote

$$\begin{aligned} \mu_{\xi+1} &\equiv m - \mathsf{rank}(A_{\mathsf{L}}) = \mathsf{dim}(\mathcal{N}(A_{\mathsf{L}}^{\mathsf{T}})), &\quad \nu_{\xi+1} &\equiv n - \mathsf{rank}(A_{\mathsf{L}}) = \mathsf{dim}(\mathcal{N}(A_{\mathsf{L}})), \\ \delta_{\zeta+1} &\equiv d - \mathsf{rank}(A_{\mathsf{R}}) = \mathsf{dim}(\mathcal{N}(A_{\mathsf{R}}^{\mathsf{T}})), & \gamma_{\zeta+1} &\equiv c - \mathsf{rank}(A_{\mathsf{R}}) = \mathsf{dim}(\mathcal{N}(A_{\mathsf{R}})). \end{aligned}$$

Thus,

$$\begin{aligned} \Sigma &= \mathsf{diag}\big(\,\sigma_1 I_{\mu_1}\,,\ \ldots\ ,\ \sigma_\xi I_{\mu_\xi}\,,\ 0_{\mu_{\xi+1},\nu_{\xi+1}}\,\big), \\ \Psi &= \mathsf{diag}\big(\,\psi_1 I_{\delta_1}\,,\ \ldots\ ,\ \psi_\zeta I_{\delta_\zeta}\,,\ 0_{\delta_{\zeta+1},\gamma_{\zeta+1}}\,\big). \end{aligned} \tag{8.5}$$

Using the SVDs, the problem (8.1) is transformed to

$$\begin{aligned} (U_{\mathsf{L}}^{\mathsf{T}} A_{\mathsf{L}} V_{\mathsf{L}})\,(V_{\mathsf{L}}^{\mathsf{T}} X V_{\mathsf{R}})\,(V_{\mathsf{R}}^{\mathsf{T}} A_{\mathsf{R}}^{\mathsf{T}} U_{\mathsf{R}}) &\approx (U_{\mathsf{L}}^{\mathsf{T}} B U_{\mathsf{R}}), \\ \Sigma\, Y\, \Psi^{\mathsf{T}} &\approx F, \end{aligned} \tag{8.6}$$

with diagonal system matrices, and where

$$Y = V_{\mathsf{L}}^{\mathsf{T}} X V_{\mathsf{R}} \in \mathbb{R}^{n\times c}, \qquad \text{and} \qquad F = U_{\mathsf{L}}^{\mathsf{T}} B U_{\mathsf{R}} \in \mathbb{R}^{m\times d}.$$

8.3.2 Partitioning and transformation of the right-hand side

In this step we want to preserve the achieved diagonal structure of system matrices, but also get as many zero rows and columns in the right-hand side as possible. In order to do that, we consider the partitioning of F w.r.t. multiplicities of singular values of A_{L} and A_{R}, i.e.,

$$F = \begin{bmatrix} F_{1,1} & \cdots & F_{1,\zeta} & F_{1,\zeta+1} \\ \vdots & \ddots & \vdots & \vdots \\ F_{\xi,1} & \cdots & F_{\xi,\zeta} & F_{\xi,\zeta+1} \\ F_{\xi+1,1} & \cdots & F_{\xi+1,\zeta} & F_{\xi+1,\zeta+1} \end{bmatrix} \in \mathbb{R}^{m\times d}, \qquad \text{where} \qquad F_{i,j} \in \mathbb{R}^{\mu_i \times \delta_j},$$

for $i = 1, \ldots, \xi, \xi+1$ and $j = 1, \ldots, \zeta, \zeta+1$. For simplicity we denote the block-rows and block-columns

$$F_{i,\bigstar} \equiv \left[\begin{array}{c} F_{i,1}, \ldots, F_{i,\zeta}, F_{i,\zeta+1} \end{array}\right] \in \mathbb{R}^{\mu_i \times d}, \qquad F_{\bigstar,j} \equiv \left[\begin{array}{c} F_{1,j} \\ \vdots \\ F_{\xi,j} \\ F_{\xi+1,j} \end{array}\right] \in \mathbb{R}^{m \times \delta_j}.$$

Let

$$\overline{\mu}_i = \mathsf{rank}(F_{i,\bigstar}) \qquad \text{and} \qquad \overline{\delta}_j = \mathsf{rank}(F_{\bigstar,j})$$

and consider (semi-economical) SVDs

$$F_{i,\bigstar} = L_{\mathsf{L},i} \left[\begin{array}{c} \Theta_{\mathsf{L},i} \\ 0_{\mu_i - \overline{\mu}_i, \overline{\mu}_i} \end{array}\right] W'^{\mathsf{T}}_{\mathsf{L},i} \qquad \text{and} \qquad F_{\bigstar,j} = W'_{\mathsf{R},j} \left[\begin{array}{cc} \Theta_{\mathsf{R},j} & 0_{\overline{\delta}_j, \delta_j - \overline{\delta}_j} \end{array}\right] L^{\mathsf{T}}_{\mathsf{R},j},$$

where

$$\begin{array}{lll} L_{\mathsf{L},i} \in \mathbb{O}_{\mu_i}, & \Theta_{\mathsf{L},i} \in \mathbb{R}^{\overline{\mu}_i \times \overline{\mu}_i}, & W'_{\mathsf{L},i} \in \mathbb{R}^{d \times \overline{\mu}_i}, \\ L_{\mathsf{R},j} \in \mathbb{O}_{\delta_j}, & \Theta_{\mathsf{R},j} \in \mathbb{R}^{\overline{\delta}_j \times \overline{\delta}_j}, & W'_{\mathsf{R},j} \in \mathbb{R}^{m \times \overline{\delta}_j}, \end{array}$$

and where, in particular:

- $\Theta_{\mathsf{L},i}$, $\Theta_{\mathsf{R},j}$ are diagonal invertible of order $\overline{\mu}_i$, $\overline{\delta}_j$, respectively, and
- $W'_{\mathsf{L},i}$, $W'_{\mathsf{R},j}$ have orthonormal columns, i.e., $W'^{\mathsf{T}}_{\mathsf{L},i} W'_{\mathsf{L},i} = I_{\overline{\mu}_i}$, $W'^{\mathsf{T}}_{\mathsf{R},j} W'_{\mathsf{R},j} = I_{\overline{\delta}_j}$,

for $i = 1, \ldots, \xi, \xi+1$ and $j = 1, \ldots, \zeta, \zeta+1$.

Define orthogonal matrices

$$\begin{aligned} L_{\mathsf{L},U} &\equiv \mathsf{diag}(L_{\mathsf{L},1}, \ldots, L_{\mathsf{L},\xi}, L_{\mathsf{L},\xi+1}) \in \mathbb{O}_m, \\ L_{\mathsf{L},V} &\equiv \mathsf{diag}(L_{\mathsf{L},1}, \ldots, L_{\mathsf{L},\xi}, I_{\nu_{\xi+1}}) \in \mathbb{O}_n, \\ L_{\mathsf{R},U} &\equiv \mathsf{diag}(L_{\mathsf{R},1}, \ldots, L_{\mathsf{R},\zeta}, L_{\mathsf{R},\zeta+1}) \in \mathbb{O}_d, \\ L_{\mathsf{R},V} &\equiv \mathsf{diag}(L_{\mathsf{R},1}, \ldots, L_{\mathsf{R},\zeta}, I_{\gamma_{\zeta+1}}) \in \mathbb{O}_c. \end{aligned}$$

Since (8.5), we have

$$L^{\mathsf{T}}_{\mathsf{L},U} \Sigma L_{\mathsf{L},V} = \Sigma \qquad \text{and} \qquad L^{\mathsf{T}}_{\mathsf{R},U} \Psi L_{\mathsf{R},V} = \Psi.$$

Thus, with the use of these matrices the problem (8.6) can be further transformed, while preserving diagonal system matrices, to

$$\begin{aligned} (L^{\mathsf{T}}_{\mathsf{L},U} \Sigma L_{\mathsf{L},V})\,(L^{\mathsf{T}}_{\mathsf{L},V} Y L_{\mathsf{R},V})\,(L^{\mathsf{T}}_{\mathsf{R},V} \Psi^{\mathsf{T}} L_{\mathsf{R},U}) &\approx (L^{\mathsf{T}}_{\mathsf{L},U} F L_{\mathsf{R},U}), \\ \Sigma\, Z\, \Psi^{\mathsf{T}} &\approx H, \end{aligned} \tag{8.7}$$

with diagonal system matrices, and where

$$Z = L^{\mathsf{T}}_{\mathsf{L},V} Y L_{\mathsf{R},V} \in \mathbb{R}^{n \times c}, \qquad \text{and} \qquad H = L^{\mathsf{T}}_{\mathsf{L},U} F L_{\mathsf{R},U} \in \mathbb{R}^{m \times d}.$$

8.3.3 Note on structure of the right-hand side

It would be useful to look at the structure of the new right-hand side of (8.7). Clearly,

$$H = L_{\mathsf{L},U}^{\mathsf{T}} F L_{\mathsf{R},U} = \left[\begin{array}{cccc} L_{\mathsf{L},1}^{\mathsf{T}} F_{1,1} L_{\mathsf{R},1} & \cdots & L_{\mathsf{L},1}^{\mathsf{T}} F_{1,\zeta} L_{\mathsf{R},\zeta} & L_{\mathsf{L},1}^{\mathsf{T}} F_{1,\zeta+1} L_{\mathsf{R},\zeta+1} \\ \vdots & \ddots & \vdots & \vdots \\ L_{\mathsf{L},\xi}^{\mathsf{T}} F_{\xi,1} L_{\mathsf{R},1} & \cdots & L_{\mathsf{L},\xi}^{\mathsf{T}} F_{\xi,\zeta} L_{\mathsf{R},\zeta} & L_{\mathsf{L},\xi}^{\mathsf{T}} F_{\xi,\zeta+1} L_{\mathsf{R},\zeta+1} \\ L_{\mathsf{L},\xi+1}^{\mathsf{T}} F_{\xi+1,1} L_{\mathsf{R},1} & \cdots & L_{\mathsf{L},\xi+1}^{\mathsf{T}} F_{\xi+1,\zeta} L_{\mathsf{R},\zeta} & L_{\mathsf{L},\xi+1}^{\mathsf{T}} F_{\xi+1,\zeta+1} L_{\mathsf{R},\zeta+1} \end{array}\right]$$

has block-rows and block-columns

$$L_{\mathsf{L},i}^{\mathsf{T}} F_{i,\bigstar} L_{\mathsf{R},U} = \left[\begin{array}{c} \Theta_{\mathsf{L},i} {W'}_{\mathsf{L},i}^{\mathsf{T}} \\ 0_{\mu_i - \overline{\mu}_i, d} \end{array}\right] L_{\mathsf{R},U}, \qquad L_{\mathsf{L},U}^{\mathsf{T}} F_{\bigstar,j} L_{\mathsf{R},j} = L_{\mathsf{L},U}^{\mathsf{T}} \left[\begin{array}{cc} W'_{\mathsf{R},j} \Theta_{\mathsf{R},j} & 0_{m,\delta_j - \overline{\delta}_j} \end{array}\right],$$

with $\overline{\mu}_i$ nonzero and mutually orthogonal rows (followed by $\mu_i - \overline{\mu}_i$ zero rows), and $\overline{\delta}_j$ nonzero and mutually orthogonal columns (followed by $\delta_j - \overline{\delta}_j$ zero columns), respectively. Thus

$$L_{\mathsf{L},i}^{\mathsf{T}} F_{i,j} L_{\mathsf{R},j} \equiv \left[\begin{array}{cc} H_{i,j} & 0_{\overline{\mu}_i, \delta_j - \overline{\delta}_j} \\ 0_{\mu_i - \overline{\mu}_i, \overline{\delta}_j} & 0_{\mu_i - \overline{\mu}_i, \delta_j - \overline{\delta}_j} \end{array}\right], \qquad H_{i,j} \in \mathbb{R}^{\overline{\mu}_i \times \overline{\delta}_j}.$$

Moreover, note that block-rows and block-columns

$$\left[\begin{array}{c} H_{i,1}, \ldots, H_{i,\zeta}, H_{i,\zeta+1} \end{array}\right] \in \mathbb{R}^{\overline{\mu}_i \times (\sum_{j=1}^{\zeta+1} \overline{\delta}_j)}, \qquad \left[\begin{array}{c} H_{1,j} \\ \vdots \\ H_{\xi,j} \\ H_{\xi+1,j} \end{array}\right] \in \mathbb{R}^{(\sum_{i=1}^{\xi+1} \overline{\mu}_i) \times \overline{\delta}_j},$$

are of *full row rank, having mutually orthogonal rows* for $i = 1, \ldots, \xi, \xi+1$, and of *full column rank, having mutually orthogonal columns* for $j = 1, \ldots, \zeta, \zeta+1$.

8.3.4 Final permutation

Now we again want to aggregate the relevant information revealed in the nonzero blocks of the right-hand side H. This can be done by a pair of permutation matrices

$$\Pi_{\mathsf{L},U} \equiv \left[\begin{array}{ccc|ccc} \left[\begin{smallmatrix} I_{\overline{\mu}_1} \\ 0 \end{smallmatrix}\right] & 0 & 0 & \left[\begin{smallmatrix} 0 \\ I_{\mu_1 - \overline{\mu}_1} \end{smallmatrix}\right] & 0 & 0 \\ & \ddots & \vdots & & \ddots & \vdots \\ 0 & \left[\begin{smallmatrix} I_{\overline{\mu}_\xi} \\ 0 \end{smallmatrix}\right] & 0 & 0 & \left[\begin{smallmatrix} 0 \\ I_{\mu_\xi - \overline{\mu}_\xi} \end{smallmatrix}\right] & 0 \\ 0 \quad \cdots & 0 & \left[\begin{smallmatrix} I_{\overline{\mu}_{\xi+1}} \\ 0 \end{smallmatrix}\right] & 0 \quad \cdots & 0 & \left[\begin{smallmatrix} 0 \\ I_{\mu_{\xi+1} - \overline{\mu}_{\xi+1}} \end{smallmatrix}\right] \end{array}\right] \in \mathbb{O}_m,$$

$$\Pi_{\mathsf{R},U} \equiv \left[\begin{array}{cccc|cccc} \left[\begin{smallmatrix} I_{\overline{\delta}_1} \\ 0 \end{smallmatrix}\right] & & 0 & 0 & \left[\begin{smallmatrix} 0 \\ I_{\delta_1-\overline{\delta}_1} \end{smallmatrix}\right] & & 0 & 0 \\ & \ddots & & \vdots & & \ddots & & \vdots \\ 0 & & \left[\begin{smallmatrix} I_{\overline{\delta}_\zeta} \\ 0 \end{smallmatrix}\right] & 0 & 0 & & \left[\begin{smallmatrix} 0 \\ I_{\delta_\zeta-\overline{\delta}_\zeta} \end{smallmatrix}\right] & 0 \\ 0 & \cdots & 0 & \left[\begin{smallmatrix} I_{\overline{\delta}_{\zeta+1}} \\ 0 \end{smallmatrix}\right] & 0 & \cdots & 0 & \left[\begin{smallmatrix} 0 \\ I_{\delta_{\zeta+1}-\overline{\delta}_{\zeta+1}} \end{smallmatrix}\right] \end{array}\right] \in \mathbb{O}_d,$$

since

$$\Pi_{\mathsf{L},U}^{\mathsf{T}} H \Pi_{\mathsf{R},U} = \Pi_{\mathsf{L},U}^{\mathsf{T}} \begin{bmatrix} \begin{bmatrix} H_{1,1} & 0 \\ 0 & 0 \end{bmatrix} & \cdots & \begin{bmatrix} H_{1,\zeta} & 0 \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} H_{1,\zeta+1} & 0 \\ 0 & 0 \end{bmatrix} \\ \vdots & \ddots & \vdots & \vdots \\ \begin{bmatrix} H_{\xi,1} & 0 \\ 0 & 0 \end{bmatrix} & \cdots & \begin{bmatrix} H_{\xi,\zeta} & 0 \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} H_{\xi,\zeta+1} & 0 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} H_{\xi+1,1} & 0 \\ 0 & 0 \end{bmatrix} & \cdots & \begin{bmatrix} H_{\xi+1,\zeta} & 0 \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} H_{\xi+1,\zeta+1} & 0 \\ 0 & 0 \end{bmatrix} \end{bmatrix} \Pi_{\mathsf{R},U}$$

$$= \left[\begin{array}{cccc|c} H_{1,1} & \cdots & H_{1,\zeta} & H_{1,\zeta+1} & \\ \vdots & \ddots & \vdots & \vdots & \\ H_{\xi,1} & \cdots & H_{\xi,\zeta} & H_{\xi,\zeta+1} & 0_{m,d-\overline{d}} \\ H_{\xi+1,1} & \cdots & H_{\xi+1,\zeta} & H_{\xi+1,\zeta+1} & \\ \hline \multicolumn{4}{c|}{0_{m-\overline{m},d-\overline{d}}} & 0_{m-\overline{m},d-\overline{d}} \end{array}\right] = \begin{bmatrix} B_1 & 0_{m,d-\overline{d}} \\ 0_{m-\overline{m},d-\overline{d}} & 0_{m-\overline{m},d-\overline{d}} \end{bmatrix},$$

where $\overline{m} = \sum_{i=1}^{\xi+1} \overline{\mu}_i$ and $\overline{d} = \sum_{j=1}^{\zeta+1} \overline{\delta}_j$. We see that we interpret the leading principle nonzero submatrix of $(\Pi_{\mathsf{L},U}^{\mathsf{T}} H \Pi_{\mathsf{R},U})$ as

$$B_1 \in \mathbb{R}^{\overline{m} \times \overline{n}},$$

i.e., the core problem right-hand side matrix; see (8.4).

Similarly as in the tensor right-hand side case (see Section 7.3.5), multiplication of the whole approximation problem by both permutation matrices

$$(\Pi_{\mathsf{L},U}^{\mathsf{T}}\, \Sigma)\, Z\, (\Psi^{\mathsf{T}}\, \Pi_{\mathsf{R},U}) \approx \Pi_{\mathsf{L},U}^{\mathsf{T}} H \Pi_{\mathsf{R},U}$$

results in shuffling the diagonal structure of the system matrices Σ and Ψ. In order to get matrices in block-diagonal form with diagonal blocks we employ two other permutation matrices

$$\Pi_{\mathsf{L},V} \equiv \left[\begin{array}{ccc|cccc} \left[\begin{smallmatrix} I_{\overline{\mu}_1} \\ 0 \end{smallmatrix}\right] & & 0 & \left[\begin{smallmatrix} 0 \\ I_{\mu_1-\overline{\mu}_1} \end{smallmatrix}\right] & & 0 & 0 \\ & \ddots & & & \ddots & & \vdots \\ 0 & & \left[\begin{smallmatrix} I_{\overline{\mu}_\xi} \\ 0 \end{smallmatrix}\right] & 0 & & \left[\begin{smallmatrix} 0 \\ I_{\mu_\xi-\overline{\mu}_\xi} \end{smallmatrix}\right] & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & I_{\nu_{\xi+1}} \end{array}\right] \in \mathbb{O}_n,$$

$$\Pi_{\mathsf{R},V} \equiv \left[\begin{array}{ccc|cccc} \begin{bmatrix} I_{\bar{\delta}_1} \\ 0 \end{bmatrix} & & 0 & \begin{bmatrix} 0 \\ I_{\delta_1 - \bar{\delta}_1} \end{bmatrix} & & 0 & 0 \\ & \ddots & & & \ddots & & \vdots \\ 0 & & \begin{bmatrix} I_{\bar{\delta}_\zeta} \\ 0 \end{bmatrix} & 0 & & \begin{bmatrix} 0 \\ I_{\delta_\zeta - \bar{\delta}_\zeta} \end{bmatrix} & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & I_{\gamma_{\zeta+1}} \end{array}\right] \in \mathbb{O}_c.$$

Then, similarly as in (7.11),

$$\Pi_{\mathsf{L},U}^{\mathsf{T}} \, \Sigma \, \Pi_{\mathsf{L},V} \equiv \begin{bmatrix} A_{\mathsf{L},11} & 0 \\ 0 & A_{\mathsf{L},22} \end{bmatrix}, \qquad \Pi_{\mathsf{R},U}^{\mathsf{T}} \, \Psi \, \Pi_{\mathsf{R},V} \equiv \begin{bmatrix} A_{\mathsf{R},11} & 0 \\ 0 & A_{\mathsf{R},22} \end{bmatrix},$$

is the wanted block-diagonal structure; see (8.4).

8.3.5 Summary of the reduction

Let us summarize the whole reduction. Starting with (8.1) we proceed: transformation based on SVD of the system matrix (8.6), right-hand side decomposition (8.7), and final permutation. In total we get

$$\Big((\Pi_{\mathsf{L},U}^{\mathsf{T}} L_{\mathsf{L},U}^{\mathsf{T}} U_{\mathsf{L}}^{\mathsf{T}}) \, A_{\mathsf{L}} \, (V_{\mathsf{L}} L_{\mathsf{L},V} \Pi_{\mathsf{L},V}) \Big) \Big((\Pi_{\mathsf{L},V}^{\mathsf{T}} L_{\mathsf{L},V}^{\mathsf{T}} V_{\mathsf{L}}^{\mathsf{T}}) \, X \, (V_{\mathsf{R}} L_{\mathsf{R},V} \Pi_{\mathsf{R},V}) \Big)$$
$$\Big((\Pi_{\mathsf{R},V}^{\mathsf{T}} L_{\mathsf{R},V}^{\mathsf{T}} V_{\mathsf{R}}^{\mathsf{T}}) \, A_{\mathsf{R}}^{\mathsf{T}} \, (U_{\mathsf{R}} L_{\mathsf{R},U} \Pi_{\mathsf{R},U}) \Big) \approx \Big((\Pi_{\mathsf{L},U}^{\mathsf{T}} L_{\mathsf{L},U}^{\mathsf{T}} U_{\mathsf{L}}^{\mathsf{T}}) \, B \, (U_{\mathsf{R}} L_{\mathsf{R},U} \Pi_{\mathsf{R},U}) \Big),$$

i.e.,

$$\begin{bmatrix} A_{\mathsf{L},11} & 0 \\ 0 & A_{\mathsf{L},22} \end{bmatrix} \widetilde{X} \begin{bmatrix} A_{\mathsf{R},11} & 0 \\ 0 & A_{\mathsf{R},22} \end{bmatrix}^{\mathsf{T}} \approx \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix},$$

the core problem revealing transformation (8.3), (8.4). Clearly,

$$P = U_{\mathsf{L}} L_{\mathsf{L},U} \Pi_{\mathsf{L},U}, \quad Q = V_{\mathsf{L}} L_{\mathsf{L},V} \Pi_{\mathsf{L},V}, \quad R = V_{\mathsf{R}} L_{\mathsf{R},V} \Pi_{\mathsf{R},V}, \quad \text{and} \quad K = U_{\mathsf{R}} L_{\mathsf{R},U} \Pi_{\mathsf{R},U},$$

and

$$\overline{m} = \sum_{i=1}^{\xi+1} \overline{\mu}_i, \quad \overline{n} = \sum_{i=1}^{\xi} \overline{\mu}_i, \quad \overline{d} = \sum_{j=1}^{\zeta+1} \overline{\delta}_j, \quad \text{and} \quad \overline{c} = \sum_{j=1}^{\zeta} \overline{\delta}_j.$$

The minimality of this construction is discussed in [9]; see also [6].

8.4 PROPERTIES OF CORE PROBLEM WITHIN $A_L X A_R^{\mathsf{T}} \approx B$

The above described core problem reduction guarantees the following properties of the core problem

$$A_{\mathsf{L},11} X_{11} A_{\mathsf{R},11}^{\mathsf{T}} \approx B_1$$

within the bilinear problem with matrix right-hand side (see [9]):

$*$(CP1) $A_{\mathsf{L},11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of *full column rank* equal to $\overline{n}$, and
$A_{\mathsf{R},11} \in \mathbb{R}^{\overline{d}\times\overline{c}}$ is of *full column rank* equal to $\overline{c}$.

$*$(CP2) $B_1 U_{\mathsf{R},j} \in \mathbb{R}^{\overline{m}\times\overline{\delta}_j}$ are of *full column rank* equal to $\overline{\delta}_j$, for $j = 1, \ldots, \overline{\zeta}, \overline{\zeta}+1$.

$*$(CP3) $U_{\mathsf{L},i}^{\mathsf{T}} B_1 \in \mathbb{R}^{\overline{\mu}_i\times\overline{d}}$ are of *full row rank* equal to $\overline{\mu}_i$, for $i = 1, \ldots, \overline{\xi}, \overline{\xi}+1$.

(CP4) $[B_1, A_{\mathsf{L},11}] \in \mathbb{R}^{\overline{m}\times(\overline{n}+\overline{d})}$ is of *full row rank* equal to $\overline{m}$, and
$[B_1^{\mathsf{T}}, A_{\mathsf{R},11}] \in \mathbb{R}^{\overline{d}\times(\overline{c}+\overline{m})}$ is of *full row rank* equal $\overline{d}$.

Columns of $U_{\mathsf{L},i}$ form the basis of the ith left singular vector subspaces of $A_{\mathsf{L},11}$ (including the null-space of $A_{\mathsf{L},11}^{\mathsf{T}}$), and columns of $U_{\mathsf{R},j}$ form the basis of the jth left singular vector subspaces of $A_{\mathsf{R},11}$ (including the null-space of $A_{\mathsf{R},11}^{\mathsf{T}}$). Three properties which are asterisked are again in fact equivalent to the minimality of such subproblem. For more interesting properties of the core problem see in particular [9] and [11, Appendix A].

Remark 7 (on TLS solvability). *The bilinear (core) problem with matrix right-hand side is a matrix approximation problem (there are no tensors of higher orders), however, the TLS theory for such problems is (up to the knowledge of the author) not done yet; see also Remark 6. Consequently, we do not know whether such core problem does or does not have the (possibly unique) TLS solution. TLS solvability is analyzed only (i) for* $d = c = 1$ *— the vector right-hand side problems (see [2], [22]); and (ii) for* $d = c$ *with* $A_{\mathsf{R}} = I_d$ *and with fixed* $E_{\mathsf{R}} = 0_{d,d}$ *— the matrix right-hand side problems (see [30], [5]).*

9 MULTILINEAR (OR k-LINEAR) PROBLEM WITH TENSOR RIGHT-HAND SIDE

The most general variant of linear approximation problems can be achieved by the combination of the two preceding cases, where there is a tensor right-hand side and multilinear mapping. This yields in the k-linear problem with tensor right-hand side. Related results have been recently published in [11]; see also the enclosed copy on page 187.

9.1 PROBLEM FORMULATION AND THE TLS MINIMIZATION

By the k-linear approximation problem we understand

$$(A_1, \ldots, A_k \,|\, \mathcal{X}) \approx \mathcal{B}, \qquad A_s \in \mathbb{R}^{m_s \times n_s},\ \mathcal{X} \in \mathbb{R}^{n_1 \times \cdots \times n_k},\ \mathcal{B} \in \mathbb{R}^{m_1 \times \cdots \times m_k}, \tag{9.1}$$

where $s = 1, \ldots, k$; see [11]. By solving such problem in the TLS sense, i.e., by the TLS method, we understand solving the following minimization problem

$$\min_{\substack{\mathcal{G} \in \mathbb{R}^{m_1 \times \cdots \times m_k} \\ E_1 \in \mathbb{R}^{m_1 \times n_1} \\ \vdots \\ E_k \in \mathbb{R}^{m_k \times n_k}}} \left(\|\mathcal{G}\|^2 + \sum\nolimits_{s=1}^{k} \|E_s\|_F^2 \right)^{\frac{1}{2}} \tag{9.2}$$

$$\text{subject to} \qquad \exists\, \mathcal{X}_{\mathsf{TLS}} \in \mathbb{R}^{n_1 \times \cdots \times n_k} \;:\; (A_1 + E_1, \ldots, A_k + E_k \,|\, \mathcal{X}_{\mathsf{TLS}}) = \mathcal{B} + \mathcal{G}.$$

We call it the k-linear TLS problem with tensor right-hand side.

Remark 8 (on TLS solvability)**.** *Similarly to the bilinear case (see Remark 6), results on TLS solvability generalizing the classification from [5] are not known to the author. The question of TLS solvability of bilinear and k-linear TLS problems remains open. It is, however, out of the scope of this thesis.*

9.2 CORE PROBLEM WITHIN $(A_1,\dots,A_k\,|\,\mathcal{X})\approx\mathcal{B}$

When we want to extract the core problem within k-linear problem (9.1), we again seek for orthogonal transformation, now realized by $2k$ orthogonal matrices

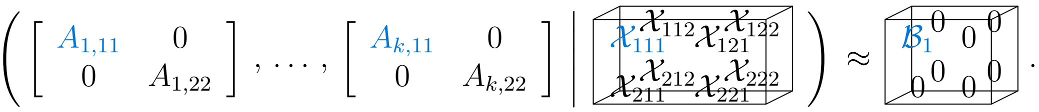
$$(P_1,Q_1,\dots,P_k,Q_k)\in\mathbb{O}_{m_1}\times\mathbb{O}_{n_1}\times\cdots\times\mathbb{O}_{m_k}\times\mathbb{O}_{n_k}.$$

The corresponding TLS minimization stays unchanged under transformation

$$\Big(P_1^{\mathsf T}A_1Q_1\,,\,\dots\,,\,P_k^{\mathsf T}A_kQ_k\,\Big|\,(Q_1^{\mathsf T},\dots,Q_k^{\mathsf T}\,|\,\mathcal{X})\Big)\approx(P_1^{\mathsf T},\dots,P_k^{\mathsf T}\,|\,\mathcal{B}) \qquad (9.3)$$

due to the orthogonal invariance of the employed norms.

The goal is to find such orthogonal transformation yielding a block diagonal structure of the problem (tensors illustrated as being of order three for clarity)



(9.4)

The original problem is, therefore, partitioned into 2^k subproblems, in particular,

$$(A_{1,11},\dots,A_{k,11}\,|\,\mathcal{X}_{1\dots1})\approx\mathcal{B}_1,\ \ A_{s,11}\in\mathbb{R}^{\overline{m}_s\times\overline{n}_s},\ \ \mathcal{X}_{11\dots1}\in\mathbb{R}^{\overline{n}_1\times\cdots\times\overline{n}_k},\ \ \mathcal{B}_1\in\mathbb{R}^{\overline{m}_1\times\dots\times\overline{m}_k},$$

where $s=1,\dots,k$, and

$$(A_{1,i_1i_1},\dots,A_{k,i_ki_k}\,|\,\mathcal{X}_{i_1\dots i_k})\approx0,\qquad(i_1,\dots,i_k)\in\Big(\{1,2\}^k\setminus(1,\dots,1)\Big).$$

The only subproblem we need to solve is the first one; the others obviously have zero solutions. The first subproblem with minimal dimensions (among all possible orthogonal transformations yielding this block structure) is called the core problem; see [11].

9.3 CORE PROBLEM REDUCTION FOR $(A_1,\dots,A_k\,|\,\mathcal{X})\approx\mathcal{B}$

In this section we summarize the process of core problem reduction for the multilinear problem with tensor right-hand side. This reduction was already published in [11] (notation in the paper differs from the notation here; we prefer simplicity in the paper, whereas consistency among individual reductions here). It generalizes the procedure of the core problem reductions published in [8] (see Section 7.3) and in [9] (see Section 8.3). The procedure again consists of three steps:

- Transformation of the system matrices (Section 9.3.1).
- Partitioning and transformation of the right-hand side (Section 9.3.2).
- Final permutation (Section 9.3.4).

The right-hand side preprocessing is again done implicitly.

9.3.1 Transformation of the system matrices

Similarly to the bilinear problem, we start with SVDs of all system matrices and we transform them into diagonal forms, i.e.,

$$A_s = U_s \Sigma_s V_s^{\mathsf{T}}, \qquad U_s \in \mathbb{O}_{m_s}, \quad \Sigma_s \in \mathbb{R}^{m_s \times n_s}, \quad V \in \mathbb{O}_{n_s}, \qquad \text{for} \quad s = 1, \ldots, k.$$

Let A_s have ξ_s distinct nonzero singular values

$$\sigma_{s,1} > \sigma_{s,2} > \cdots > \sigma_{s,\xi_s} > 0,$$

and let μ_{s,i_s}, $i_s = 1, \ldots, \xi_s$, be their multiplicities, i.e.,

$$\sum_{i_s=1}^{\xi_s} \mu_{s,i_s} = \mathrm{rank}(A_s).$$

Further denote

$$\mu_{s,\xi_s+1} \equiv m_s - \mathrm{rank}(A_s) = \dim(\mathcal{N}(A_s^{\mathsf{T}})), \quad \nu_{s,\xi_s+1} \equiv n_s - \mathrm{rank}(A_s) = \dim(\mathcal{N}(A_s)).$$

Thus

$$\Sigma_s = \mathrm{diag}\big(\sigma_{s,1} I_{\mu_{s,1}}\,,\ \ldots\ ,\ \sigma_{s,\xi_s} I_{\mu_{s,\xi_s}}\,,\ 0_{\mu_{s,\xi_s+1},\nu_{s,\xi_s+1}}\big), \quad \text{for} \quad s = 1, \ldots, k. \tag{9.5}$$

Employing these SVDs, the original problem (9.1) is transformed to

$$\begin{aligned} \Big(U_1^{\mathsf{T}} A_1 V_1, \ldots, U_k^{\mathsf{T}} A_k V_k \,\Big|\, \big(V_1^{\mathsf{T}}, \ldots, V_k^{\mathsf{T}} \,\big|\, \mathcal{X} \big) \Big) &\approx \big(U_1^{\mathsf{T}}, \ldots, U_k^{\mathsf{T}} \,\big|\, \mathcal{B} \big), \\ \big(\Sigma_1, \ldots, \Sigma_k \,\big|\, \mathcal{Y} \big) &\approx \mathcal{F}, \end{aligned} \tag{9.6}$$

with diagonal system matrices, and where

$$\begin{aligned} \mathcal{Y} &= \big(V_1^{\mathsf{T}}, \ldots, V_k^{\mathsf{T}} \,\big|\, \mathcal{X} \big) \in \mathbb{R}^{n_1 \times \cdots \times n_k}, \quad \text{and} \\ \mathcal{F} &= \big(U_1^{\mathsf{T}}, \ldots, U_k^{\mathsf{T}} \,\big|\, \mathcal{B} \big) \in \mathbb{R}^{m_1 \times \cdots \times m_k}. \end{aligned}$$

9.3.2 Partitioning and transformation of the right-hand side

In this step we again want to transform the right-hand side tensor such that: we preserve the achieved diagonal structure of system matrices, and we also get as many zero blocks (in the form of whole zero fibres) in the right-hand side tensor as possible. In order to do that, we consider the partitioning of $\mathcal{F}$ w.r.t. multiplicities of singular values of A_s, i.e.,

$$\mathcal{F}^{\{s\}} = \begin{bmatrix} F_{s,1} \\ \vdots \\ F_{s,\xi_s} \\ F_{s,\xi_s+1} \end{bmatrix} \in \mathbb{R}^{m_s \times (\Delta_{\mathcal{F}}/m_s)}, \qquad \text{where} \qquad F_{s,i_s} \in \mathbb{R}^{\mu_{s,i_s} \times (\Delta_{\mathcal{F}}/m_s)},$$

for $i_s = 1, \ldots, \xi_s, \xi_s + 1$ and $s = 1, \ldots, k$, and where $\Delta_{\mathcal{F}} = \prod_{\ell=1}^{k} m_\ell$. Tensor $\mathcal{F}$ is, therefore, partitioned into a grid of

$$(\xi_1 + 1) \times \cdots \times (\xi_k + 1)$$

sub-tensors

$$\mathcal{F}_{i_1,\cdots,i_k} \in \mathbb{R}^{\mu_{1,i_1} \times \cdots \times \mu_{k,i_k}},$$

for $i_s = 1, \ldots, \xi_s, \xi_s + 1$ and $s = 1, \ldots, k$. (Matrix F_{s,i_s} contains s-mode fibres of all sub-tensors $\mathcal{F}_{i_1,\cdots,i_k}$ with the sth index fixed to the value i_s, sorted in the inverse lexicographical order w.r.t. their multi-indices.) Let

$$\overline{\mu}_{s,i_s} = \text{rank}(F_{s,i_s})$$

and consider (semi-economical) SVDs

$$F_{s,i_s} = L_{s,i_s} \begin{bmatrix} \Theta_{s,i_s} \\ 0_{\mu_{s,i_s} - \overline{\mu}_{s,i_s}, \overline{\mu}_{s,i_s}} \end{bmatrix} W'^{\mathsf{T}}_{s,i_s},$$

where

$$L_{s,i_s} \in \mathbb{O}_{\mu_{i_s}}, \quad \Theta_{s,i_s} \in \mathbb{R}^{\overline{\mu}_{s,i_s} \times \overline{\mu}_{s,i_s}}, \quad W'_{s,i_s} \in \mathbb{R}^{(\Delta_{\mathcal{F}}/m_s) \times \overline{\mu}_{s,i_s}},$$

and where, in particular:

- Θ_{s,i_s} are diagonal invertible of order $\overline{\mu}_{s,i_s}$, and
- W'_{s,i_s} have orthonormal columns, i.e., $W'^{\mathsf{T}}_{s,i_s} W'_{s,i_s} = I_{\overline{\mu}_{s,i_s}}$,

for $i_s = 1, \ldots, \xi_s, \xi_s + 1$ and $s = 1, \ldots, k$.

Define orthogonal matrices

$$\begin{aligned} L_{s,U} &\equiv \text{diag}(L_{s,1}, \ldots, L_{s,\xi_s}, L_{s,\xi_s+1}) \in \mathbb{O}_{m_s}, \\ L_{s,V} &\equiv \text{diag}(L_{s,1}, \ldots, L_{s,\xi_s}, I_{\nu_{s,\xi_s+1}}) \in \mathbb{O}_{n_s}, \end{aligned}$$

Since (9.5),

$$L_{s,U}^{\mathsf{T}} \, \Sigma_s \, L_{s,V} = \Sigma_s, \qquad \text{for} \quad s = 1, \ldots, k,$$

the problem (9.6) can be further transformed, while preserving diagonal system matrices to

$$\begin{aligned} \Big(L_{1,U}^{\mathsf{T}} \Sigma_1 L_{1,V}, \ldots, L_{k,U}^{\mathsf{T}} \Sigma_k L_{k,V} \,\Big|\, \big(L_{1,V}^{\mathsf{T}}, \ldots, L_{k,V}^{\mathsf{T}} \,\big|\, \mathcal{Y} \big) \Big) &\approx \big(L_{1,U}^{\mathsf{T}}, \ldots, L_{k,U}^{\mathsf{T}} \,\big|\, \mathcal{F} \big), \\ \big(\Sigma_1, \ldots, \Sigma_k \,\big|\, \mathcal{Z} \big) &\approx \mathcal{H}, \end{aligned} \tag{9.7}$$

with diagonal system matrices, and where

$$\begin{aligned} \mathcal{Z} &= \big(L_{1,V}^{\mathsf{T}}, \ldots, L_{k,V}^{\mathsf{T}} \,\big|\, \mathcal{Y} \big) \in \mathbb{R}^{n_1 \times \cdots \times n_k}, \quad \text{and} \\ \mathcal{H} &= \big(L_{1,U}^{\mathsf{T}}, \ldots, L_{k,U}^{\mathsf{T}} \,\big|\, \mathcal{F} \big) \in \mathbb{R}^{m_1 \times \cdots \times m_k}. \end{aligned}$$

9.3.3 Note on structure of the right-hand side

It would be useful to look at the structure of the new right-hand side of (9.7). Employing the s-mode matricization (see [15]), we get

$$\mathcal{H}^{\{s\}} = L_{s,U}^{\mathsf{T}}\, \mathcal{F}^{\{s\}} \underbrace{\Big((L_{k,U} \otimes \cdots \otimes L_{s+1,U}) \otimes (L_{s-1,U} \otimes \cdots \otimes L_{1,U}) \Big)}_{\Lambda_s \,\in\, \mathbb{O}_{\Delta_{\mathcal{F}}/m_s}}$$

$$= \begin{bmatrix} L_{s,1}^{\mathsf{T}} F_{s,1} \\ \vdots \\ L_{s,\xi_s}^{\mathsf{T}} F_{s,\xi_s} \\ L_{s,\xi_s+1}^{\mathsf{T}} F_{s,\xi_s+1} \end{bmatrix} \Lambda_s,$$

where $\otimes$ is the Kronecker product. This matricization has block-rows of the form

$$L_{s,i_s}^{\mathsf{T}} F_{s,i_s} = \begin{bmatrix} \Theta_{s,i_s} {W'}_{s,i_s}^{\mathsf{T}} \\ 0_{\mu_{s,i_s} - \overline{\mu}_{s,i_s}, \Delta_{\mathcal{F}}/m_s} \end{bmatrix} \Lambda_s$$

with $\overline{\mu}_{s,i_s}$ nonzero and mutually orthogonal rows (followed by $\mu_{s,i_s} - \overline{\mu}_{s,i_s}$ zero rows), for all $s = 1, \ldots, k$. In terms of the grid of sub-tensors we get

$$\big(\, L_{1,i_1}^{\mathsf{T}}, \ldots, L_{k,i_k}^{\mathsf{T}} \,\big|\, \mathcal{F}_{i_1,\cdots,i_k} \,\big) \equiv \mathrm{diag}_k(\mathcal{H}_{i_1,\cdots,i_k}, 0_{\mu_{1,i_1} - \overline{\mu}_{1,i_1}, \ldots, \mu_{k,i_k} - \overline{\mu}_{k,i_k}}),$$

where

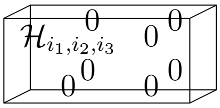
$$\mathcal{H}_{i_1,\cdots,i_k} \in \mathbb{R}^{\overline{\mu}_{1,i_1} \times \cdots \times \overline{\mu}_{k,i_k}}.$$

Moreover, note that a matrix formed as block-row of s-mode matricizations of all $\mathcal{H}_{i_1,\cdots,i_k}$ tensors with the given fixed value i_s of the sth index is of full row rank equal to $\overline{\mu}_{s,i_s}$ having mutually orthogonal rows, for all $i_s = 1, \ldots, \xi_s, \xi_s + 1$ and $s = 1, \ldots, k$.

9.3.4 Final permutation

Similarly as in previous two cases (see Sections 7.3.5 and 8.3.4). Tensor $\mathcal{H}$ (of dimensions $\times_{s=1}^{k} m_s$) consists of the regular grid of sub-tensor (of dimensions $\times_{s=1}^{k} \mu_{s,j_s}$) with nonzero leading principal parts $\mathcal{H}_{i_1,\cdots,i_k}$ (of dimensions $\times_{s=1}^{k} \overline{\mu}_{s,j_s}$); illustration for $s = 3$:

$$\big(\, L_{1,i_1}^{\mathsf{T}}, L_{2,i_2}^{\mathsf{T}}, L_{3,i_3}^{\mathsf{T}} \,\big|\, \mathcal{F}_{i_1,i_2,i_3} \,\big) =$$



.

The final step collects all the blocks $\mathcal{H}_{i_1,\cdots,i_k}$ together in the leading principal corner of the whole tensor, while forming $\mathcal{B}_1$ there. It is again realized by permutation matrices $\Pi_{s,U} \equiv$

$$\left[\begin{array}{cccc|cccc} \begin{bmatrix} I_{\overline{\mu}_{s,1}} \\ 0 \end{bmatrix} & & 0 & 0 & \begin{bmatrix} 0 \\ I_{\mu_{s,1}-\overline{\mu}_{s,1}} \end{bmatrix} & & 0 & 0 \\ & \ddots & & \vdots & & \ddots & & \vdots \\ 0 & & \begin{bmatrix} I_{\overline{\mu}_{s,\xi_s}} \\ 0 \end{bmatrix} & 0 & 0 & & \begin{bmatrix} 0 \\ I_{\mu_{s,\xi_s}-\overline{\mu}_{s,\xi_s}} \end{bmatrix} & 0 \\ 0 & \cdots & 0 & \begin{bmatrix} I_{\overline{\mu}_{s,\xi_s+1}} \\ 0 \end{bmatrix} & 0 & \cdots & 0 & \begin{bmatrix} 0 \\ I_{\mu_{s,\xi_s+1}-\overline{\mu}_{s,\xi_s+1}} \end{bmatrix} \end{array}\right]$$

of order m_s, for $s = 1, \ldots, k$. Then

$$\left(\Pi_{1,U}^{\mathsf{T}}, \ldots, \Pi_{kk,U}^{\mathsf{T}} \,\middle|\, \mathcal{H} \right) = \mathrm{diag}_k(\mathcal{B}_1 \,,\, 0_{m_1-\overline{m}_1,\ldots,m_k-\overline{m}_k}),$$

where $\overline{m}_s = \sum_{i_s=1}^{\xi_s+1} \overline{\mu}_{s,i_s}$. The leading principal block

$$\mathcal{B}_1 \in \mathbb{R}^{\overline{m}_1 \times \cdots \times \overline{m}_k}$$

is the core problem right-hand side tensor; see (9.4).

Application of all these permutations on the whole approximation problem again shuffle diagonality of all system matrices Σ_s. Their structure cannot be fully restored in general, but they can be permuted into block-diagonal form with diagonal blocks — again by employing permutation matrices

$$\Pi_{s,V} \equiv \left[\begin{array}{ccc|cccc} \begin{bmatrix} I_{\overline{\mu}_{s,1}} \\ 0 \end{bmatrix} & & 0 & \begin{bmatrix} 0 \\ I_{\mu_{s,1}-\overline{\mu}_{s,1}} \end{bmatrix} & & 0 & 0 \\ & \ddots & & & \ddots & & \vdots \\ 0 & & \begin{bmatrix} I_{\overline{\mu}_{s,\xi_s}} \\ 0 \end{bmatrix} & 0 & & \begin{bmatrix} 0 \\ I_{\mu_{s,\xi_s}-\overline{\mu}_{s,\xi_s}} \end{bmatrix} & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & I_{\nu_{s,\xi_s+1}} \end{array}\right] \in \mathbb{O}_{n_s}.$$

Then similarly as in (7.11)

$$\Pi_{s,U}^{\mathsf{T}} \, \Sigma_s \, \Pi_{s,V} \equiv \begin{bmatrix} A_{s,11} & 0 \\ 0 & A_{s,22} \end{bmatrix}$$

is the wanted block-diagonal structure; see (9.4).

9.3.5 Summary of the reduction

Let us summarize the whole reduction. Starting with (9.1) we proceed: transformation based on SVD of the system matrix (9.6), right-hand side decomposition (9.7), and final permutation. In total we get

$$\Bigg((\Pi_{1,U}^{\mathsf{T}} L_{1,U}^{\mathsf{T}} U_1^{\mathsf{T}}) \, A_1 \, (V_1 L_{1,V} \Pi_{1,V}) \,, \, \ldots \,, \, (\Pi_{k,U}^{\mathsf{T}} L_{k,U}^{\mathsf{T}} U_k^{\mathsf{T}}) \, A_k \, (V_k L_{k,V} \Pi_{k,V}) \Bigg|$$

$$\left((\Pi_{1,V}^{\mathsf{T}} L_{1,V}^{\mathsf{T}} V_1^{\mathsf{T}}) \,, \, \ldots \,, \, (\Pi_{k,V}^{\mathsf{T}} L_{k,V}^{\mathsf{T}} V_k^{\mathsf{T}}) \,\middle|\, \mathcal{X} \right) \Bigg) \approx \left((\Pi_{1,U}^{\mathsf{T}} L_{1,U}^{\mathsf{T}} U_1^{\mathsf{T}}) \,, \, \ldots \,, \, (\Pi_{k,U}^{\mathsf{T}} L_{k,U}^{\mathsf{T}} U_k^{\mathsf{T}}) \,\middle|\, \mathcal{B} \right)$$

i.e.,

$$\left(\begin{bmatrix} A_{1,11} & 0 \\ 0 & A_{1,22} \end{bmatrix}, \dots, \begin{bmatrix} A_{k,11} & 0 \\ 0 & A_{k,22} \end{bmatrix} \,\middle|\, \widetilde{\mathcal{X}}\right) \approx \mathrm{diag}_k(\mathcal{B}_1, 0_{m_1-\overline{m}_1,\dots,m_k-\overline{m}_k}),$$

the core problem revealing transformation (9.3), (9.4). Clearly,

$$P_s = U_s L_{s,U} \Pi_{s,U}, \quad \text{and} \quad Q_s = V_s L_{s,V} \Pi_{s,V}, \quad \text{for} \quad s = 1, \dots, k,$$

and

$$\overline{m}_s = \sum_{i_s=1}^{\xi_s+1} \overline{\mu}_{s,i_s}, \quad \text{and} \quad \overline{n}_s = \sum_{i_s=1}^{\xi_s} \overline{\mu}_{s,i_s}, \quad \text{for} \quad s = 1, \dots, k.$$

The minimality of this construction is discussed in [11]; see also [6].

9.4 PROPERTIES OF CORE PROBLEM WITHIN $(A_1, \dots, A_k \,|\, \mathcal{X}) \approx \mathcal{B}$

The procedure of the core problem reduction again guarantees the properties of core problem

$$(A_{1,11}, \dots, A_{k,11} \,|\, \mathcal{X}_{1\dots1}) \approx \mathcal{B}_1,$$

within k-linear problem with tensor right-hand side (see [11]), for $s = 1, \dots, k$:

$*$(CP1) $A_{s,11} \in \mathbb{R}^{\overline{m}_s \times \overline{n}_s}$ are of *full column rank* equal to $\overline{n}_s$.

$*$(CP2–3) $U_{s,i_s}^{\mathsf{T}} \mathcal{B}_1^{\{s\}} \in \mathbb{R}^{\overline{\mu}_{s,i_s} \times (\Delta_{\mathcal{B}_1}/\overline{m}_s)}$ are of *full row rank* $\overline{\mu}_{s,i_s}$, for $i_s = 1, \dots, \overline{\xi}_s, \overline{\xi}_s + 1$.

(CP4) $[\mathcal{B}_1^{\{s\}}, A_{s,11}] \in \mathbb{R}^{\overline{m}_s \times (\overline{n}_s + \Delta_{\mathcal{B}_1}/\overline{m}_s)}$ are of *full row rank* equal to $\overline{m}_s$.

Recall that $\Delta_{\mathcal{B}_1} = \prod_{\ell=1}^{k} \overline{m}_\ell$, and columns of U_{s,i_s} form the basis of the i_sth left singular vector subspaces of $A_{s,11}$ (including the null-space of $A_{s,11}^{\mathsf{T}}$). Again, the two asterisked properties are equivalent to the minimality of such subproblem. For further properties of this core problem see in particular [11].

Remark 9 (on TLS solvability)**.** *Discussion about potential TLS solvability of such core problem is fully open, since the TLS theory for multilinear approximation problem is (up to the knowledge of the author) not done yet; see also Remark 8. It is done only (i) for $k = 1$ (or equivalently $d_2 = \cdots = d_k = 1$) — the vector right-hand side problems (see [2], [22]); and (ii) for $k = 2$ (or equivalently $d_3 = \cdots = d_k = 1$) with $m_2 = n_2$, $A_2 = I_{n_2}$, and with fixed $E_2 = 0_{n_2,n_2}$ — the matrix right-hand side problems (see [30], [5]).*

MAJOR PUBLISHED RESULTS RELATED TO THE PART III

1. I. Hnětynková, M. Plešinger, and J. Žáková, *TLS formulation and core reduction for problems with structured right-hand sides*, Linear Algebra and its Applications 555 (2018), pp. 241–265.

   `https://www.sciencedirect.com/science/article/pii/S0024379518303008`

   See also page 141, or reference [8].
2. I. Hnětynková, M. Plešinger, and J. Žáková, *On TLS formulation and core reduction for data fitting with generalized models*, Linear Algebra and its Applications 577 (2019), pp. 1–20.

   `https://www.sciencedirect.com/science/article/pii/S0024379519301703`

   See also page 167, or reference [9].
3. I. Hnětynková, M. Plešinger, and J. Žáková, *Krylov subspace approach to core problems within multilinear approximation problems: A unifying framework*, SIAM Journal on Matrix Analysis and Applications 44 (1) (2023), pp. 53–79.

   `https://epubs.siam.org/doi/abs/10.1137/21M1462155`

   See also page 187, or reference [11].

Linear Algebra and its Applications 555 (2018) 241–265

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

TLS formulation and core reduction for problems with structured right-hand sides [☆]

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A R T I C L E I N F O

Article history:
Received 6 December 2017
Accepted 13 June 2018
Available online 18 June 2018
Submitted by B. Meini

MSC:
15A09
15A21
15A69
65F20
65F25

Keywords:
Total least squares problem (TLS)
Error-in-variables modeling
Orthogonal regression
Tensor decomposition
Core problem

A B S T R A C T

The total least squares (TLS) represents a popular data fitting approach for solving linear approximation problems $Ax \approx b$ (i.e., with a vector right-hand side) and $AX \approx B$ (i.e., with a matrix right-hand side) contaminated by errors. This paper introduces a generalization of TLS formulation to problems with structured right-hand sides. First, we focus on the case, where the right-hand side and consequently also the solution are tensors. We show that whereas the basic solvability result can be obtained directly by matricization of both tensors, generalization of the core problem reduction is more complicated. The core reduction allows to reduce mathematically the problem dimensions by removing all redundant and irrelevant data from the system matrix and the right-hand side. We prove that the core problems within the original tensor problem and its matricized counterpart are in general different. Then, we concentrate on problems with even more structured right-hand sides, where the same model A corresponds to a set of various tensor right-hand

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[☆] This work has been partially supported by the SGS grant of Technical University of Liberec No. 21254/2018, by the scholarship of The Preciosa Foundation, and by the GACR grant No. 17-04150J.

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https://doi.org/10.1016/j.laa.2018.06.016

sides. Finally, relations between the matrix and tensor core problem are discussed.

1. Introduction

Let $\mathscr{U}$ and $\mathscr{V}$ be finite-dimensional linear (vector) spaces over the same field $\mathbb{F}$. Typically $\mathscr{U}$ and $\mathscr{V}$ are spaces of column vectors or matrices over the field of real ($\mathbb{R}$) or complex ($\mathbb{C}$) numbers. Let $\mathcal{A} \in \mathscr{L}(\mathscr{U}, \mathscr{V})$ be a linear mapping, $\mathcal{A} : \mathscr{U} \longrightarrow \mathscr{V}$, with the range $\mathscr{R}(\mathcal{A}) \subseteq \mathscr{V}$. Consider the approximation problem

$$\mathcal{A}(x) \approx b, \qquad \text{where} \qquad x \in \mathscr{U}, \quad b \in \mathscr{V} \tag{1.1}$$

are the *unknown vector* and the *right-hand side (observation) vector*, respectively. Assume that $b \notin \mathscr{R}(\mathcal{A})$, i.e., the problem does not have a solution in the classical meaning. If the data $\mathcal{A}$ and/or b are contaminated by errors, various data correction techniques are used to solve (1.1). The *total least squares (TLS)* approach is very general, since it allows for corrections in both $\mathcal{A}$ and b by seeking for a perturbation (or correction) g of the right-hand side b, and for a perturbation (or correction) $\mathcal{E}$ of the mapping $\mathcal{A}$ so that

$$\min_{\substack{g \in \mathscr{V} \\ \mathcal{E} \in \mathscr{E} \subseteq \mathscr{L}(\mathscr{U}, \mathscr{V})}} \|(g, \mathcal{E})\|_{\star} \qquad \text{subject to} \qquad (\mathcal{A} + \mathcal{E})(x) = b + g, \tag{1.2}$$

where $\|\cdot\|_{\star}$ denotes some norm in $\mathscr{V} \times \mathscr{L}(\mathscr{U}, \mathscr{V})$, and $(\mathcal{A} + \mathcal{E})(x) \equiv \mathcal{A}(x) + \mathcal{E}(x)$. Note that $\mathscr{E}$, the *search set* for the mapping perturbation $\mathcal{E}$, is either the whole space $\mathscr{L}(\mathscr{U}, \mathscr{V})$, or its proper subspace (or submanifold) depending on the problem (1.1). Any vector x which solves the perturbed problem (1.2) is called the *TLS solution*. In the case that the TLS solution is not unique, we are often interested in the solution minimal with respect to some norm $\|\cdot\|_{\diamond}$ in $\mathscr{U}$.

The TLS (and also closely related orthogonal regression and errors-in-variables modeling) has been widely used to solve problems (1.1) in two most common forms: The *single* and *multiple right-hand side* problems, where b is either a column vector or a matrix, and $\mathcal{A}$ is a matrix; see for example [35, Chap. 1], [33], or [34]. It is well known that even in the single right-hand side case the TLS problem may not have a solution; see the analysis in [4], [35] and also [5, Chap. 6.3]. The so-called core problem theory introduced in [21] provided an alternative view on TLS problems by showing how redundant and irrelevant data can be removed from $\mathcal{A}$ and b. This allowed to clarify why TLS problems may not have a solution and what is the meaning of the nongeneric solutions defined in [35]. The solvability analysis of the multiple (matrix) right-hand side case started in [35] has been complemented in [7]. Recently, also generalization of the core problem theory has been derived in a sequence of papers [9], [10], [6]. However, many questions still remain open.

In many practical cases the problem underlying (1.1) (and therefore also its solution) depends on one or more parameters that impose some further structure into the data; see for example [23] where the mapping depends on a vector of parameters, or [18] where the right-hand side depends on time. TLS problems originated in noise and error-contaminated dynamical systems (see [25]) naturally depend on time; dynamical systems depending on more parameters can be found, e.g., in the Oberwolfach collection [16]. Assume the simplest case, where the right-hand side vector b depends on several (let say $k-1$) parameters $\lambda_2, \lambda_3, \ldots, \lambda_k$. Each of the parameters λ_j is sampled in some region of interest to d_j samples and we have in hands the observation b on the regular Cartesian grid of these samples. If b is an m-vector, the whole set of observations form a k-way tensor $\mathcal{B}$, a hyperblock of entries of dimensions $m \times d_2 \times \cdots \times d_k$; see for example [13] or [12] for the same approach in a different context. This yields naturally a problem (1.1) of the form

$$\mathcal{A}(\mathcal{X}) \equiv A \times_1 \mathcal{X} \approx \mathcal{B}, \tag{1.3}$$

where A is a matrix, $\mathcal{X}$ and $\mathcal{B}$ are *tensors of unknowns and right-hand sides*, respectively, and "$\times_1$" stands for a *matrix-tensor product* that will be specified later in section 3.1; see (3.2). (Note that, for a general linear approximation problem $\mathcal{A}(\mathcal{X}) \approx \mathcal{B}$ the mapping may also be a tensor of appropriate dimensions; analysis of this general case is however out of the scope of this paper and will be presented elsewhere.) The problem (1.3) can be trivially reshaped (matricized) into a matrix problem, and solved by standard matrix methods including the TLS. However, in this paper we show mathematically that leaving the tensor structure (imposed by the parameters) of the data may not be appropriate.

Overview of our contributions: We formulate the TLS minimization within (1.3) in a tensor form. We show that although the basic TLS solvability results can then be obtained directly by matricization of (1.3), this is not true for the core problem representing the *necessary and sufficient information* within (1.3). By employing the so-called Tucker decomposition of the right-hand side tensor $\mathcal{B}$, we prove that there always exists the tensor shaped core problem that preserves the imposed structure. We develop an explicit unitary transformation revealing this tensor core problem. Then we show that the tensor core problem is in general different from its counterpart obtained from the matricization of (1.3). Finally, the results are extended to problems with even more structured right-hand sides called the coupled TLS problems. This formulation could be appropriate for example when the observations are not available for the full Cartesian grid, and the missing columns are avoided, e.g., by cutting the incomplete hyperblock into some set of its mutually disjoint subtensors. Presented results may be useful in solving of approximation problems with structured right-hand sides, where the least squares techniques are heavily employed (see, e.g., [27]). Since the introduced tensor formulation covers also the formulations analyzed previously, we believe it can help with understanding of some of the open questions related to standard TLS problems.

The organization of the paper is the following. Section 2 briefly summarizes the classical (vector and matrix right-hand side) TLS formulations. Section 3 recalls some basic definitions related to tensors. Section 4 introduces the tensor right-hand side TLS problem and derives the tensorized core reduction while proving the existence and uniqueness of the obtained core problem. Section 5 generalizes the results to the coupled TLS problem—a set of several problems with the same matrix A and different tensor right-hand sides. Section 6 compares the ordinary and tensor core problem. Section 7 concludes the paper.

Throughout the paper I_ℓ (or just I) denotes an $\ell \times \ell$ identity matrix and $e_i^{(\ell)}$ (or just e_i) its ith column; $0_{\ell,\xi}$ (or just 0) denotes an $\ell \times \xi$ zero matrix; and M^{T}, $M^* \equiv \overline{M}^{\mathsf{T}}$, $\mathscr{R}(M)$, and $\mathscr{N}(M)$ denote the transposition, the Hermitian conjugation, the range, and the null-space of a matrix M, respectively. Further, $M \otimes K$ denotes the Kronecker product of matrices where $m_{i,j}$, the (i,j)th entry of M is replaced by the block $m_{i,j}K$.

2. Classical TLS formulations

In the classical setting, the mapping $\mathcal{A}$ is represented by a (generally rectangular) matrix A called the *system (or model) matrix*. We consider two cases of problems depending on the number of observations being available for this model.

2.1. Single right-hand side problem

The simplest case of (1.1) is the *single right-hand side problem* of the form

$$Ax \approx b, \qquad \text{or, equivalently,} \qquad [b, A]\begin{bmatrix} -1 \\ x \end{bmatrix} \approx 0, \tag{2.1}$$

where $A \in \mathbb{F}^{m\times n}$, $x \in \mathbb{F}^n$, and $b \in \mathbb{F}^m$. Here (1.2) is typically considered as

$$\min_{\substack{g\in\mathbb{F}^m\\ E\in\mathbb{F}^{m\times n}}} \|[g, E]\|_F \qquad \text{subject to} \qquad (A + E)x = b + g, \tag{2.2}$$

i.e., the *correction matrix* $[g, E]$ is minimized in the Frobenius norm.

Golub and Van Loan gave the sufficient condition for the existence of the unique TLS solution of (2.1)–(2.2) in [4]. Van Huffel and Vandewalle further extended the analysis and obtained the necessary and sufficient condition for the existence of any (possibly nonunique) TLS solution. They also introduced the concept of the nongeneric solution for the case when the TLS solution does not exist; see [35, Chap. 3].

The analysis was complemented by the so-called *core problem* transformation in [19], [20], and in particular [21]. Since the Frobenius norm in (2.2) is unitarily invariant, the original problem (2.1) can be transformed to

$$\widehat{A}\widehat{x} \equiv (P^*AQ)(Q^*x) \approx (P^*b) \equiv \widehat{b}, \tag{2.3}$$

where $P^{-1} = P^*$, $Q^{-1} = Q^*$ are unitary matrices; or, equivalently,

$$[\widehat{b}, \widehat{A}] \begin{bmatrix} -1 \\ \widehat{x} \end{bmatrix} \equiv \left(P^* [b, A] \begin{bmatrix} 1 & 0 \\ 0 & Q \end{bmatrix} \right) \left(\begin{bmatrix} 1 & 0 \\ 0 & Q^* \end{bmatrix} \begin{bmatrix} -1 \\ x \end{bmatrix} \right) \approx 0. \tag{2.4}$$

Paige and Strakoš showed in [21] that there always exist P and Q giving

$$[\widehat{b}, \widehat{A}] = P^* [b, A] \begin{bmatrix} 1 & 0 \\ 0 & Q \end{bmatrix} \equiv \left[\begin{array}{c|cc} b_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{array} \right], \tag{2.5}$$

where $[b_1, A_{11}]$ has minimal and A_{22} maximal dimensions over all unitary transformations yielding the block structure (2.5). Combining (2.4) and (2.5), together with conformal partitioning of $\widehat{x} = \left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]$, the original problem splits into two independent subproblems

$$A_{11} x_1 \approx b_1 \qquad \text{and} \qquad A_{22} x_2 \approx 0, \tag{2.6}$$

where only the first needs to be solved, since $x_2 = 0$.

The first problem $A_{11} x_1 \approx b_1$ is called the *core problem*. It is given uniquely (up to an unitary transformation) and it has several interesting properties; see [21]. First of all, the core problem always has the unique TLS solution. Moreover, its back-transformation

$$x = Q\widehat{x} = Q \begin{bmatrix} x_1 \\ 0 \end{bmatrix} \tag{2.7}$$

represents either the unique TLS solution of (2.1) if it exists, or the minimum norm TLS solution if (2.1) has more than one TLS solutions, or the (minimum norm) nongeneric solution if (2.1) does not have a TLS solution. In this way, the core problem reduction allows to extract the *necessary and sufficient information* for solving the original problem into a typically smaller core problem. The core problem concept also helps to explain the meaning of the nongeneric solution; see [21].

2.2. Multiple right-hand side problem

In the case that multiple observations are available, (1.1) takes the form of the *multiple right-hand side problem*

$$AX \approx B, \qquad \text{or, equivalently,} \qquad [B, A] \begin{bmatrix} -I_d \\ X \end{bmatrix} \approx 0, \tag{2.8}$$

where $A \in \mathbb{F}^{m \times n}$, $X \in \mathbb{F}^{n \times d}$, and $B \in \mathbb{F}^{m \times d}$. Here (1.2) becomes

$$\min_{\substack{G\in\mathbb{F}^{m\times d}\\ E\in\mathbb{F}^{m\times n}}} \|[G,E]\|_F \qquad \text{subject to} \qquad (A+E)X = B+G, \tag{2.9}$$

i.e., the *correction matrix* $[G,E]$ is minimized in the Frobenius norm.

Such approach was studied by Van Huffel (see [31], [32]), Van Huffel and Vandewalle (see [35, Chap. 3]), Wei (see [38] and [39]), and many others. The necessary and sufficient condition for the existence of the TLS solution of (2.8)–(2.9) was given in [7]; see also [8] and [11].

The generalization of the core problem concept was then derived in the series of papers [9], [10], and [6] (see also the first attempts in [1], [2], [24], and [22]). Since the norm used in (2.9) is unitarily invariant, the original problem (2.8) can be transformed to

$$\widehat{A}\widehat{X} \equiv (P^*AQ)(Q^*XR) \approx (P^*BR) \equiv \widehat{B}, \tag{2.10}$$

where $P^{-1} = P^*$, $Q^{-1} = Q^*$, $R^{-1} = R^*$ are unitary matrices. In [9] it has been shown, that there always exist P, Q, and R giving

$$[\widehat{B},\widehat{A}] = P^*[B,A]\begin{bmatrix} R & 0 \\ 0 & Q \end{bmatrix} \equiv \left[\begin{array}{cc|cc} B_1 & 0 & A_{11} & 0 \\ 0 & 0 & 0 & A_{22} \end{array}\right], \tag{2.11}$$

where $[B_1, A_{11}]$ has minimal and A_{22} maximal dimensions over all unitary transformations yielding the block structure (2.11). Conformal partitioning of $\widehat{X} = \left[\begin{smallmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{smallmatrix}\right]$ splits the original problem into four independent subproblems

$$A_{11}X_{11} \approx B_1 \qquad \text{and} \qquad A_{11}X_{12} \approx 0, \quad A_{22}X_{21} \approx 0, \quad A_{22}X_{22} \approx 0, \tag{2.12}$$

where only the first needs to be solved, since $X_{12} = 0$, $X_{21} = 0$, $X_{22} = 0$. The first problem $A_{11}X_{11} \approx B_1$ called the *core problem* is again given uniquely (up to an unitary transformation).

It is worth to recall that the multiple (as well as the single) right-hand side approximation problem represents a core problem if and only if it satisfies the following three characteristic properties (see [9, section 4]):

(CP1) The matrix A_{11} is of *full column rank*.
(CP2) The matrix B_1 is of *full column rank*.
(CP3) Let A_{11} have ξ distinct nonzero singular values with multiplicities μ_i and $\mu_{\xi+1} \equiv \dim(\mathcal{N}(A_{11}^*))$, and let U_i be matrices having orthonormal bases of left singular vector subspaces of A_{11} as their columns.
Then the matrices $U_i^*B_1$ are of *full row rank* μ_i, for $i = 1, \ldots, \xi, \xi+1$.

These imply several other properties (see [10] and [6]), among others:

(CP4) The extended matrix $[B_1|A_{11}]$ is of *full row rank*.

Note that some questions related to the TLS solvability in the multiple right-hand side case still remain open. For example, the multiple right-hand side core problem (contrary to the single right-hand side one) may not have a TLS solution or the TLS solution may not be unique; see [6].

2.3. Note on general unitarily invariant norms

The minimization in (2.2) and (2.9) can be considered also in other unitarily invariant norms. Ranks of the correction matrices are in both cases bounded by the number of columns in the corresponding right-hand sides, i.e., $0 \leq \operatorname{rank}([g, E]) \leq 1$ and $0 \leq \operatorname{rank}([G, E]) \leq d$, respectively. Consequently, $[g, E]$ has at most one nonzero singular value making minimizations in (2.2) for all unitarily invariant norms conceptually the same. However, in the multiple right-hand side case, at most d singular values of $[G, E]$ might be nonzero. Thus, various unitarily invariant norms in (2.9) generally lead to different minimization (e.g., employing only the largest singular value for the spectral norm $\|\cdot\|_2$, or all nonzero singular values for the Frobenius norm $\|\cdot\|_F$, etc.; see also [26, Chap. II.3] and [37]). The classification of TLS problems with respect to an arbitrary unitarily invariant norm has been introduced recently in [17] and [36].

3. From matrix to tensor setting

Now we repeat basic tensor notation useful in the following derivations. By a *tensor of order k* we understand a k-way ($k \geq 1$) array of dimensions $n_1, n_2, \ldots, n_k$ ($n_j \geq 1$, $j = 1, 2, \ldots, k$),

$$\mathcal{T} \in \mathbb{F}^{n_1 \times n_2 \times \cdots \times n_k} \qquad \text{with entries} \qquad t_{i_1, i_2, \ldots, i_k}, \tag{3.1}$$

where $\mathbb{F}$ equals $\mathbb{R}$ or $\mathbb{C}$. Its individual indices (or directions, or ways) $1, 2, \ldots, k$ are called *modes*; see, e.g., [15], [14]. The one-way and two-way tensors are called simply vectors and matrices, respectively.

Denote $n \equiv \prod_{j=1}^{k} n_j$ the total number of entries of $\mathcal{T}$. Three important types of subarrays of a tensor are:

- n/n_p subarrays in $\mathbb{F}^{1 \times \cdots \times 1 \times n_p \times 1 \times \cdots \times 1}$ called the *p-mode fibers*, trivially isomorphic with vectors of length n_p (the fibers of a two-way tensor are called the columns and rows);
- $n/(n_p n_u)$ subarrays in $\mathbb{F}^{1 \times \cdots \times 1 \times n_p \times 1 \times \cdots \times 1 \times n_u \times 1 \times \cdots \times 1}$ called the *(p, u)-modes slices*, trivially isomorphic with n_p-by-n_u matrices (the slices of a three-way tensor are called frontal, lateral, and horizontal);
- n_p subarrays in $\mathbb{F}^{n_1 \times \cdots \times n_{p-1} \times 1 \times n_{p+1} \times \cdots \times n_k}$ called the *p-mode co-fibers*, trivially isomorphic with $(k-1)$-way tensors.

3.1. The matrix-tensor product and the tensor norm

For the tensor $\mathcal{T} \in \mathbb{F}^{n_1\times n_2\times\cdots\times n_k}$ and a matrix $S \in \mathbb{F}^{m_p\times n_p}$, the *p-mode matrix-tensor product*[1] is defined as the k-way tensor

$$\begin{aligned} &\mathcal{Z} = S \times_p \mathcal{T} \in \mathbb{F}^{n_1\times\cdots\times n_{p-1}\times m_p\times n_{p+1}\times\cdots\times n_k} \\ \text{with entries} \quad &z_{i_1,i_2,\ldots,i_k} = \textstyle\sum_{\alpha=1}^{n_p} t_{i_1,\ldots,i_{p-1},\alpha,i_{p+1},\ldots,i_k}\cdot s_{i_p,\alpha}\,, \end{aligned} \tag{3.2}$$

i.e., a p-mode fiber of $\mathcal{Z}$ is obtained by multiplication of S by a p-mode fiber of $\mathcal{T}$, where the fibers are handled as vectors; see, e.g., [3], [27]. Multiplication by $S_\ell \in \mathbb{F}^{m_\ell\times n_\ell}$ in all modes $\ell = 1, 2, \ldots, k$ is for simplicity denoted as

$$[\![\mathcal{T}\,|\,S_1, S_2, \ldots, S_k]\!] \equiv S_k \times_k (\cdots \times_3 (S_2 \times_2 (S_1 \times_1 \mathcal{T}))\cdots). \tag{3.3}$$

If all S_ℓ's are invertible, (3.3) can be seen as a *linear transformation* of $\mathcal{T}$.

For a norm of $\mathcal{T}$ we consider

$$\|\mathcal{T}\| \equiv \left(\sum_{i_1=1}^{n_1}\sum_{i_2=1}^{n_2}\cdots\sum_{i_k=1}^{n_k}|t_{i_1,i_2,\ldots,i_k}|^2\right)^{\frac{1}{2}}, \tag{3.4}$$

a straightforward generalization of the Euclidean vector and Frobenius matrix norm; see [15]. Clearly, (3.4) is unitarily invariant, i.e.,

$$\|\mathcal{T}\| = \|Q_p \times_p \mathcal{T}\| = \|[\![\mathcal{T}\,|\,Q_1, Q_2, \ldots, Q_k]\!]\|, \quad \text{for} \quad Q_p^* = Q_p^{-1}, \quad p = 1, 2, \ldots, k.$$

3.2. The matricization and the vectorization

Let $\mathcal{T}$ be the tensor (3.1) and let $\mathscr{R} \equiv \{r_1, r_2, \ldots, r_R\}$, $\mathscr{C} \equiv \{c_1, c_2, \ldots, c_C\}$ be sets of indices so that $\mathscr{R}\cup\mathscr{C} = \{1, 2, \ldots, k\}$ and $\mathscr{R}\cap\mathscr{C} = \varnothing$ (i.e., $k = R+C$), and $r_1 < r_2 < \cdots < r_R$, $c_1 < c_2 < \cdots < c_C$. Then the matrix

$$\mathcal{T}^{\mathscr{R}} = \mathcal{T}^{\{r_1,r_2,\ldots,r_R\}} \in \mathbb{F}^{n_R\times n_C}, \quad \text{where} \quad n_R \equiv \textstyle\prod_{\ell=1}^{R} n_{r_\ell}\,, \quad n_C \equiv \prod_{\ell=1}^{C} n_{c_\ell}\,, \tag{3.5}$$

which contains $t_{i_1,i_2,\ldots,i_k}$ in rows with multiindices $(i_{r_R}, \ldots, i_{r_2}, i_{r_1})$ and in columns with multiindices $(i_{c_C}, \ldots, i_{c_2}, i_{c_1})$, both sorted in the lexicographical order, is called the *matricization* of $\mathcal{T}$; see, e.g., [15], [27, Chap. 3.1.2]. Clearly, $\mathcal{T}^{\mathscr{R}} = (\mathcal{T}^{\mathscr{C}})^{\mathsf{T}}$. We are particularly interested in the so-called:

- *ℓ-mode matricization* or *unfolding*, where $\mathscr{R} = \{\ell\}$, $\mathscr{C} = \{1, \ldots, k\} \setminus \{\ell\}$, and

$$\mathcal{T}^{\{\ell\}} \in \mathbb{F}^{n_\ell\times(n/n_\ell)} \tag{3.6}$$

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[1] We use the product $\times_p$ with reversed order of operands in comparison to the standard notation given in [3], to keep consistent ordering of objects in equations $Ax \approx b$, $AX \approx B$, and $A \times_1 \mathcal{X} \approx \mathcal{B}$.

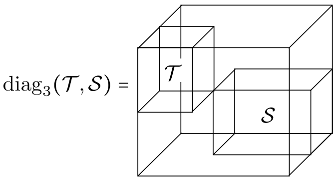

Fig. 1. The direct sum of two three-way tensors $\mathcal{T}$ and $\mathcal{S}$.

contains all the ℓ-mode fibers of $\mathcal{T}$ as columns (recall that $n = \prod_{j=1}^{k} n_j$);

- *vectorization*, where $\mathscr{R} = \{1, 2, \ldots, k\}$, $\mathscr{C} = \varnothing$, usually denoted by

$$\mathrm{vec}(\mathcal{T}) \equiv \mathcal{T}^{\{1,2,\ldots,k\}} \in \mathbb{F}^{n\times 1}, \tag{3.7}$$

which stores all the entries of $\mathcal{T}$ in one long vector.

The tensor $\mathcal{Z} = S \times_p \mathcal{T}$ (see (3.2)) can be rearranged by matricization $\mathcal{Z}^{\{p\}} = S\,\mathcal{T}^{\{p\}}$. Similarly, for (3.3) we have in general

$$[\![\mathcal{T}\,|\,S_1, S_2, \ldots, S_k]\!]^{\mathscr{R}} = (S_{r_R} \otimes \cdots \otimes S_{r_2} \otimes S_{r_1})\,\mathcal{T}^{\mathscr{R}}\,(S_{c_C} \otimes \cdots \otimes S_{c_2} \otimes S_{c_1})^{\mathsf{T}}, \tag{3.8}$$

and in particular

$$\mathrm{vec}([\![\mathcal{T}\,|\,S_1, S_2, \ldots, S_k]\!]) = (S_k \otimes \cdots \otimes S_2 \otimes S_1)\,\mathrm{vec}(\mathcal{T}), \tag{3.9}$$

where $\otimes$ is the Kronecker product of matrices.

3.3. The concatenation and the direct sum

Let $\mathcal{T}_\ell \in \mathbb{F}^{n_1\times\cdots\times n_{p-1}\times\alpha_\ell\times n_{p+1}\times n_k}$, $\ell = 1, \ldots, \xi$, be a set of k-way tensors of the same dimensions in all modes except for the pth mode. Then the k-way tensor

$$\mathcal{T} \equiv [\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_\xi]_p \in \mathbb{F}^{n_1\times\cdots\times n_{p-1}\times\alpha\times n_{p+1}\times n_k}, \quad \text{where} \quad \alpha \equiv \sum_{\ell=1}^{\xi} \alpha_\ell, \tag{3.10}$$

satisfying $\mathcal{T}^{\{p\}} = [(\mathcal{T}_1^{\{p\}})^{\mathsf{T}}, (\mathcal{T}_2^{\{p\}})^{\mathsf{T}}, \ldots, (\mathcal{T}_\xi^{\{p\}})^{\mathsf{T}}]^{\mathsf{T}}$, is called the ($p$-mode) *concatenation* of tensors $\mathcal{T}_\ell$. The concatenation represents a *direct sum of tensors in one mode*; here the p-mode.

A *direct sum* in all modes of two k-way tensors $\mathcal{T}$ and $\mathcal{S}$ of dimensions n_j and m_j, respectively, $j = 1, 2, \ldots, k$, is denoted by

$$\mathrm{diag}_k(\mathcal{T}, \mathcal{S}) = \mathcal{T} \oplus \mathcal{S} \in \mathbb{F}^{(n_1+m_1)\times(n_2+m_2)\times\cdots\times(n_k+m_k)}\,; \tag{3.11}$$

see also Fig. 1. In the case of two-way tensors (matrices) we use $\mathrm{diag}(T, S)$.

3.4. The Tucker decomposition

Let $\varrho_\ell \equiv \mathrm{rank}(\mathcal{T}^{\{\ell\}})$ be the ranks, and

$$\mathcal{T}^{\{\ell\}} = U_\ell \Sigma_\ell V_\ell^*, \qquad U_\ell = [U_\ell', U_\ell''] \in \mathbb{F}^{n_\ell \times n_\ell}, \quad U_\ell' \in \mathbb{F}^{n_\ell \times \varrho_\ell}, \quad U_\ell^* = U_\ell^{-1},$$

the singular value decompositions (SVDs) of the ℓ-mode matricizations of $\mathcal{T}$. Since the last $(n_\ell - \varrho_\ell)$ rows of $U_\ell^* \mathcal{T}^{\{\ell\}}$ are zeros, the transformation $[\![\mathcal{T} \,|\, U_1^*, U_2^*, \ldots, U_k^*]\!]$ yields nonzero entries only in the leading principal subtensor

$$\mathcal{T}_{\mathrm{core}} \equiv [\![\mathcal{T} \,|\, {U_1'}^*, {U_2'}^*, \ldots, {U_k'}^*]\!] \in \mathbb{F}^{\varrho_1 \times \varrho_2 \times \cdots \times \varrho_k} \tag{3.12}$$

called the *Tucker core*[2] of $\mathcal{T}$; see [28], [29], [30]; see also [15, Sec. 4.1] and [27, Chap. 3.1.2]. The uniquely given size of the Tucker core $\mathrm{rank}(\mathcal{T}) \equiv (\varrho_1, \varrho_2, \ldots, \varrho_k)$ is called the *multilinear* (or *vector*) *rank* of $\mathcal{T}$; see, e.g., [15, Sec. 3]. Finally,

$$\mathcal{T} = [\![\mathrm{diag}_k(\mathcal{T}_{\mathrm{core}}, 0) \,|\, U_1, U_2, \ldots, U_k]\!] = [\![\mathcal{T}_{\mathrm{core}} \,|\, U_1', U_2', \ldots, U_k']\!] \tag{3.13}$$

is called the (full and economic, respectively) *Tucker decomposition* of $\mathcal{T}$. It can be seen as a generalization of the (full and economic) SVD to tensors, but the Tucker core is in general full.[3]

4. TLS with tensor right-hand side

In this main part of the paper we first generalize the TLS formulation to problems with a tensor right-hand side and discuss its solvability. Then we derive the core problem transformation. We consider a linear approximation problem

$$A \times_1 \mathcal{X} \approx \mathcal{B}, \quad \text{where} \quad A \in \mathbb{F}^{m \times n}, \quad \mathcal{X} \in \mathbb{F}^{n \times d_2 \times \cdots \times d_k}, \quad \mathcal{B} \in \mathbb{F}^{m \times d_2 \times \cdots \times d_k}; \tag{4.1}$$

see also the illustration in Fig. 2.

4.1. Definition and basic solvability result

We introduce the following definition.

Definition 4.1 *(TLS with tensor right-hand side).* Let $A \times_1 \mathcal{X} \approx \mathcal{B}$ be the approximation problem (4.1). The minimization problem

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[2] Similarity in the terminology "*Tucker core*" and "*core problem*" is just a coincidence, it does not refer to any relation between these two concepts.

[3] A two-way tensor (i.e., a matrix) with the (full and economic) SVD $T = U\Sigma V^* = U'\Sigma' V'^*$, $\Sigma = \mathrm{diag}(\Sigma', 0)$, has the Tucker decomposition of the form $T = [\![\Sigma \,|\, U, \overline{V}]\!] = [\![\Sigma' \,|\, U', \overline{V'}]\!]$, i.e., $\Sigma = [\![T \,|\, U^*, V^{\mathsf{T}}]\!]$, and the Tucker core equals $\Sigma' = [\![T \,|\, U'^*, V'^{\mathsf{T}}]\!]$.

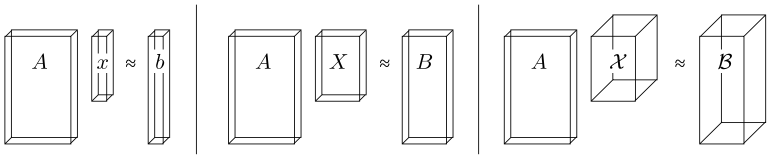


Fig. 2. Illustration of linear approximation problems with a matrix A and various right-hand sides. Left: The vector (single) right-hand side. Middle: The matrix (multiple) right-hand side. Right: The tensor (of order 3) right-hand side.

$$\min_{\substack{\mathcal{G} \in \mathbb{F}^{m \times d_2 \times \cdots \times d_k} \\ E \in \mathbb{F}^{m \times n}}} (\|\mathcal{G}\|^2 + \|E\|_F^2)^{\frac{1}{2}} \quad \text{subject to} \quad (A + E) \times_1 \mathcal{X} = \mathcal{B} + \mathcal{G} \tag{4.2}$$

is called the tensor right-hand side TLS.

Since the matricization represents only a reshaping of the array,

$$(\|\mathcal{G}\|^2 + \|E\|_F^2)^{\frac{1}{2}} = (\|\mathcal{G}^{\{1\}}\|_F^2 + \|E\|_F^2)^{\frac{1}{2}} = \|[\mathcal{G}^{\{1\}}, E]\|_F.$$

Thus we can immediately formulate a trivial but important theorem relating the tensor right-hand side TLS problem with a particular matrix right-hand side TLS problem.

Theorem 4.2. *Let (4.1)–(4.2) be a tensor right-hand side TLS problem. Consider the matrix right-hand side TLS problem (2.8)–(2.9) with*

$$X \equiv \mathcal{X}^{\{1\}} \in \mathbb{F}^{n \times d}, \quad B \equiv \mathcal{B}^{\{1\}}, \quad G \equiv \mathcal{G}^{\{1\}} \in \mathbb{F}^{n \times d}, \quad \text{and} \quad d \equiv \prod\nolimits_{j=2}^{k} d_j, \tag{4.3}$$

i.e., X, B, and G are obtained as 1-mode matricizations of tensors $\mathcal{X}$, $\mathcal{B}$, and $\mathcal{G}$, respectively. Then these two TLS problems are equivalent in the sense that X represents a TLS solution of (2.8)–(2.9) if and only if $\mathcal{X}$ represents a TLS solution of (4.1)–(4.2). Moreover, $\|X\|_F = \|\mathcal{X}\|$.

The theorem directly implies that the basic results on the existence and uniqueness of minimal corrections E and G, and of the TLS solution X obtained previously for matrix right-hand side TLS problems (see the summary in section 2) can be transferred through the equivalent formulation also to the tensor case. Moreover, the minimum F-norm TLS solution of the matrix formulation (2.8)–(2.9) with (4.3) equals the TLS solution of the tensor formulation (4.1)–(4.2) minimal in the tensor norm (3.4). Consequently, from the TLS-solvability point of view, problems with tensor right-hand side behave the same way as the matrix right-hand side problems. However, generalization of the core problem concept is significantly more complicated. First we derive the tensor core problem, its relations to matrix core problem is discussed in section 6.

4.2. Revealing the core problem

Now we derive the reduction. Basic structure of the individual steps is similar to multiple right-hand side core problem determination in [9], but requires special attention. Since both the matrix Frobenius norm and the tensor norm (3.4) in (4.2) are unitarily invariant, the original problem (4.1) can be transformed to

$$\widehat{A} \times_1 \widehat{\mathcal{X}} \equiv (P^* A Q) \times_1 [\![\mathcal{X} \,|\, Q^*, R_2^*, \dots, R_k^*]\!] \approx [\![\mathcal{B} \,|\, P^*, R_2^*, \dots, R_k^*]\!] \equiv \widehat{\mathcal{B}}, \tag{4.4}$$

where $P^{-1} = P^*$, $Q^{-1} = Q^*$, $R_j^{-1} = R_j^*$, $j = 2, \dots, k$ are unitary matrices.[4] We are looking for a transformation giving

$$[\![\mathcal{B} \,|\, P^*, R_2^*, \dots, R_k^*]\!] \equiv \mathrm{diag}_k(\mathcal{B}_1, 0), \qquad P^* A Q \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix}, \tag{4.5}$$

where both $\mathcal{B}_1$ and A_{11} have minimal dimensions over all unitary transformations yielding the block structure (4.5), and the 1-mode fibers of $\mathcal{B}_1$ are of the same length as columns of A_{11}. For such transformation, conformal partitioning of $\widehat{\mathcal{X}}$ would split the original problem to 2^k subproblems

$$\begin{aligned} A_{11} \times_1 \mathcal{X}_{1,1,\dots,1} &\approx \mathcal{B}_1, & A_{11} \times_1 \mathcal{X}_{1,i_2,\dots,i_k} &\approx 0, \\ A_{22} \times_1 \mathcal{X}_{2,1,\dots,1} &\approx 0, & A_{22} \times_1 \mathcal{X}_{2,i_2,\dots,i_k} &\approx 0, \\ (i_2, \dots, i_k) &\in \{1,2\}^{k-1}, & (i_2, \dots, i_k) &\neq (1, \dots, 1), \end{aligned} \tag{4.6}$$

where only the first called the *tensor core problem* needs to be solved, since the others have trivial solutions. We reveal the core problem in four subsequent steps described in the following sections:

4.2.1 Preprocessing of the right-hand side;
4.2.2 Transformation of the system matrix;
4.2.3 Transformation of the right-hand side;
4.2.4 Final permutation.

4.2.1. Preprocessing of the right-hand side

Let $(\delta_1, \delta_2, \dots, \delta_k) = \mathrm{rank}(\mathcal{B})$ be the multilinear rank of $\mathcal{B}$, and

$$\mathcal{B} = [\![\mathrm{diag}_k(\mathcal{B}_{\mathrm{core}}, 0) \,|\, R_1, R_2, \dots, R_k]\!] = [\![\mathcal{B}_{\mathrm{core}} \,|\, R_1', R_2', \dots, R_k']\!] \tag{4.7}$$

---

[4] Here we are not fully consistent with the core problem revealing transformation introduced for the matrix right-hand problems. The transformations of X and B in (2.10)–(2.11) become in the tensor notation $\widehat{X} = [\![X \,|\, Q^*, (\overline{R})^*]\!]$ and $\widehat{B} = [\![B \,|\, P^*, (\overline{R})^*]\!]$, respectively. In particular, R becomes $\overline{R}$; see (3.3) and also the footnote 3 on page 250.

be its Tucker decomposition, i.e., $\mathcal{B}_{\mathrm{core}} \in \mathbb{F}^{\delta_1 \times \delta_2 \times \cdots \times \delta_k}$. Then

$$A \times_1 [\![\mathcal{X} \,|\, I_n, R_2^*, \ldots, R_k^*]\!] \approx [\![\mathcal{B} \,|\, I_m, R_2^*, \ldots, R_k^*]\!] \tag{4.8}$$

with conformal partitioning of the tensor of unknowns (as before) splits the original problem to 2^{k-1} subproblems. Only the first subproblem

$$A \times_1 \mathcal{Y} \approx \mathcal{C}, \tag{4.9}$$

where

$$\begin{aligned} &\mathcal{C} \equiv [\![\mathcal{B} \,|\, I_m, {R_2'}^*, \ldots, {R_k'}^*]\!] = [\![\mathcal{B}_{\mathrm{core}} \,|\, R_1', I_{\delta_2}, \ldots, I_{\delta_k}]\!] \in \mathbb{F}^{m \times \delta_2 \times \cdots \times \delta_k} \quad \text{and} \\ &\mathcal{Y} \equiv [\![\mathcal{X} \,|\, I_n, {R_2'}^*, \ldots, {R_k'}^*]\!] \in \mathbb{F}^{n \times \delta_2 \times \cdots \times \delta_k}, \end{aligned} \tag{4.10}$$

has a nonzero right-hand side and thus needs to be solved. The other subproblems have trivial solutions. Moreover, ℓ-mode matricizations of the right-hand side $\mathcal{C}$ for $\ell = 2, \ldots, k$ are of *full row rank having mutually orthogonal rows.*

4.2.2. Transformation of the system matrix

Consider the SVD of A,

$$A = U \Sigma V^*, \qquad U \in \mathbb{F}^{m \times m}, \quad \Sigma \in \mathbb{R}^{m \times n}, \quad V \in \mathbb{F}^{n \times n}, \tag{4.11}$$

where $U^* = U^{-1}$, $V^* = V^{-1}$. Let A have ξ *distinct* nonzero singular values

$$\sigma_1 > \sigma_2 > \cdots > \sigma_\xi > 0, \tag{4.12}$$

and let m_ℓ, $\ell = 1, \ldots, \xi$, be their multiplicities, i.e., $\sum_{\ell=1}^{\xi} m_\ell = \mathrm{rank}(A)$. Further denote $m_{\xi+1} \equiv m - \mathrm{rank}(A) = \dim(\mathcal{N}(A^*))$, and $n_{\xi+1} \equiv n - \mathrm{rank}(A) = \dim(\mathcal{N}(A))$. Then

$$\Sigma = \mathrm{diag}(\sigma_1 I_{m_1}, \sigma_2 I_{m_2}, \ldots, \sigma_\xi I_{m_\xi}, 0_{m_{\xi+1}, n_{\xi+1}}). \tag{4.13}$$

The problem (4.9)–(4.10) can be transformed to

$$(U^* A V) \times_1 \mathcal{Z} = \Sigma \times_1 \mathcal{Z} \approx \mathcal{F}, \tag{4.14}$$

where

$$\begin{aligned} &\mathcal{F} \equiv [\![\mathcal{C} \,|\, U^*, I_{\delta_2}, \ldots, I_{\delta_k}]\!] = [\![\mathcal{B} \,|\, U^*, {R_2'}^*, \ldots, {R_k'}^*]\!] \quad \text{and} \\ &\mathcal{Z} \equiv [\![\mathcal{Y} \,|\, V^*, I_{\delta_2}, \ldots, I_{\delta_k}]\!] = [\![\mathcal{X} \,|\, V^*, {R_2'}^*, \ldots, {R_k'}^*]\!]. \end{aligned} \tag{4.15}$$

All ℓ-mode matricizations of $\mathcal{F}$ for $\ell = 2, \ldots, k$ are of *full row rank having mutually orthogonal rows.* The system matrix on the left of (4.14) is *diagonal.*

4.2.3. Transformation of the right-hand side

Now we focus on the 1-mode matricization of the right-hand side. From (4.14) we obtain

$$\Sigma \mathcal{Z}^{\{1\}} \approx \mathcal{F}^{\{1\}} = U^* \mathcal{C}^{\{1\}} = U^* \mathcal{B}^{\{1\}} \left(\overline{R'_k} \otimes \cdots \otimes \overline{R'_2} \right), \tag{4.16}$$

where $\mathcal{F}^{\{1\}}$ has $d \equiv (\prod_{j=2}^{k} \delta_j)$ columns. In order to get as many zero rows in the right-hand side as possible (while preserving the diagonal structure of the system matrix) we consider the following partitioning

$$\mathcal{F}^{\{1\}} = \left[F_1^{\mathsf{T}}, F_2^{\mathsf{T}}, \ldots, F_\xi^{\mathsf{T}}, F_{\xi+1}^{\mathsf{T}} \right]^{\mathsf{T}}, \quad \text{where} \quad F_\ell \in \mathbb{F}^{m_\ell \times d}, \quad \ell = 1, 2, \ldots, \xi, \xi + 1. \tag{4.17}$$

Let $\mu_\ell \equiv \operatorname{rank}(F_\ell)$. Consider the SVD of F_ℓ in the form

$$F_\ell = S_\ell \Theta_\ell W_\ell^*, \qquad S_\ell \in \mathbb{F}^{m_\ell \times m_\ell}, \quad \Theta_\ell \in \mathbb{R}^{m_\ell \times \mu_\ell}, \quad W_\ell \in \mathbb{F}^{d \times \mu_\ell}, \tag{4.18}$$

where $S_\ell^* = S_\ell^{-1}$ is square unitary, Θ_ℓ is of full column rank, and W_ℓ has mutually orthonormal columns, i.e., $W_\ell^* W_\ell = I_{\mu_\ell}$, $\ell = 1, 2, \ldots, \xi, \xi + 1$. Consider unitary matrices

$$S_U \equiv \operatorname{diag}(S_1, S_2, \ldots, S_\xi, S_{\xi+1}), \quad S_V \equiv \operatorname{diag}(S_1, S_2, \ldots, S_\xi, I_{n_{\xi+1}}). \tag{4.19}$$

Since $S_U^* \Sigma S_V = \Sigma$ (see (4.13)), the problem (4.16) can be transformed to

$$(S_U^* \Sigma S_V)(S_V^* \mathcal{Z}^{\{1\}}) = \Sigma (S_V^* \mathcal{Z}^{\{1\}}) \approx (S_U^* \mathcal{F}^{\{1\}}), \tag{4.20}$$

while preserving the diagonal structure of the system matrix. The right-hand side is then

$$S_U^* \mathcal{F}^{\{1\}} = \left[(S_1^* F_1)^{\mathsf{T}}, (S_2^* F_2)^{\mathsf{T}}, \ldots, (S_\xi^* F_\xi)^{\mathsf{T}}, (S_{\xi+1}^* F_{\xi+1})^{\mathsf{T}} \right]^{\mathsf{T}},$$

where

$$S_\ell^* F_\ell = \Theta_\ell W_\ell^* \equiv \begin{bmatrix} H_\ell \\ 0_{m_\ell - \mu_\ell, d} \end{bmatrix}, \qquad \text{with} \qquad H_\ell \in \mathbb{F}^{\mu_\ell \times d}. \tag{4.21}$$

Thus the right-hand side has the *full row rank* and *mutually orthogonal rows.*

Consequently, in the tensor notation, the problem (4.14)–(4.15) is transformed to

$$\underbrace{(S_U^* U^* A V S_V)}_{\Sigma} \times_1 [\![\mathcal{Z} \,|\, S_V^*, I_{\delta_2}, \ldots, I_{\delta_k}]\!] \approx [\![\mathcal{F} \,|\, S_U^*, I_{\delta_2}, \ldots, I_{\delta_k}]\!]. \tag{4.22}$$

The right-hand side tensor $[\![\mathcal{F} \,|\, S_U^*, I_{\delta_2}, \ldots, I_{\delta_k}]\!]$ is the 1-mode concatenation of $\xi + 1$ tensors $\mathcal{F}_\ell \in \mathbb{F}^{m_\ell \times \delta_2 \times \cdot \times \delta_k}$ satisfying $\mathcal{F}_\ell^{\{1\}} \equiv S_\ell^* F_\ell$ (see (3.10)), i.e., it contains these tensors

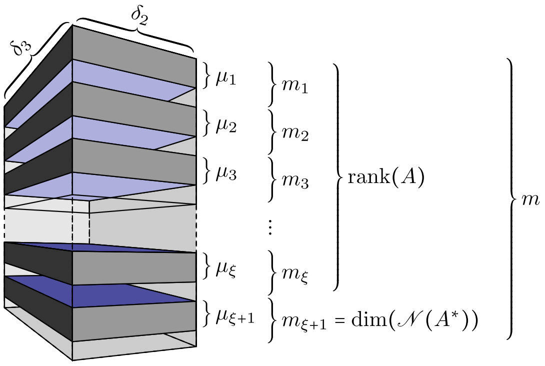


Fig. 3. The structure of the right-hand side tensor $[\![\mathcal{F} \,|\, S_U^*, I_{\delta_2}, \ldots, I_{\delta_k}]\!]$ of (4.22), for $k = 3$. The tensor contains nonzero and zero blocks concatenated along the 1-mode fibers. Each nonzero block $\mathcal{H}_\ell$, $\ell = 1, 2, \ldots, \xi, \xi + 1$, contains μ_ℓ linearly independent and mutually orthogonal horizontal slices (1-mode co-fibers in general).

as blocks concatenated along the 1-mode fibers. Each $\mathcal{F}_\ell$ block, $\ell = 1, 2, \ldots, \xi, \xi + 1$, contains two subblocks

$$\mathcal{H}_\ell \in \mathbb{F}^{\mu_\ell \times \delta_2 \times \cdots \times \delta_k} \qquad \text{and} \qquad 0 \in \mathbb{F}^{(m_\ell - \mu_\ell) \times \delta_2 \times \cdots \times \delta_k} \tag{4.23}$$

concatenated along the 1-mode fibers. The first subblock satisfies $H_\ell \equiv \mathcal{H}_\ell^{\{1\}}$ and it is formed by μ_ℓ linearly independent and mutually orthogonal 1-mode co-fibers; see Fig. 3 for illustration of the structure of the right-hand side. Note that $0 \leq \mu_\ell \leq \min\{m_\ell, d\}$ and $0 \leq (m_\ell - \mu_\ell) \leq m_\ell$, thus in particular one of the subblocks (4.23) may have no co-fibers.

4.2.4. Final permutation

Now the aim is to find a permutation of (4.22) in order to get the block structure (4.5). The permutation is given by the structure of (non)zero blocks in the right-hand side. Such permutation moves the nonzero blocks of the tensor $[\![\mathcal{F} \,|\, S_U^*, I_{\delta_2}, \ldots, I_{\delta_k}]\!]$ (or block-rows of the matrix $S_U^* \mathcal{F}^{\{1\}}$) up along the 1-mode fibers while moving the zero blocks (or block-rows) down. It can be realized by the permutation matrix

$$\Pi_U \equiv \left[\begin{array}{cccc|cccc} \begin{bmatrix} I_{\mu_1} \\ 0 \end{bmatrix} & & 0 & 0 & \begin{bmatrix} 0 \\ I_{m_1-\mu_1} \end{bmatrix} & & 0 & 0 \\ & \ddots & & \vdots & & \ddots & & \vdots \\ 0 & & \begin{bmatrix} I_{\mu_\xi} \\ 0 \end{bmatrix} & 0 & 0 & & \begin{bmatrix} 0 \\ I_{m_\xi-\mu_\xi} \end{bmatrix} & 0 \\ 0 & \cdots & 0 & \begin{bmatrix} I_{\mu_{\xi+1}} \\ 0 \end{bmatrix} & 0 & \cdots & 0 & \begin{bmatrix} 0 \\ I_{m_{\xi+1}-\mu_{\xi+1}} \end{bmatrix} \end{array}\right],$$

since

$$\Pi_U^{\mathsf{T}} (S_U^* \mathcal{F}^{\{1\}}) = \left[H_1^{\mathsf{T}}, H_2^{\mathsf{T}}, \ldots, H_\xi^{\mathsf{T}}, H_{\xi+1}^{\mathsf{T}}, 0_{d,m-\mu} \right]^{\mathsf{T}}, \quad \text{where} \quad \mu \equiv \textstyle\sum_{\ell=1}^{\xi+1} \mu_\ell. \tag{4.24}$$

Because the permutation Π_U is applied on the whole problem (4.22) from the left, the blocks in the system matrix can be permuted in an inconvenient way. This can be fixed by a second permutation applied from the right to get the block structure (4.5) of the system matrix, i.e.,

$$\Pi_V \equiv \left[\begin{array}{ccc|cccc} \begin{bmatrix} I_{\mu_1} \\ 0 \end{bmatrix} & & 0 & \begin{bmatrix} 0 \\ I_{m_1-\mu_1} \end{bmatrix} & & 0 & 0 \\ & \ddots & & & \ddots & & \vdots \\ 0 & & \begin{bmatrix} I_{\mu_\xi} \\ 0 \end{bmatrix} & 0 & & \begin{bmatrix} 0 \\ I_{m_\xi-\mu_\xi} \end{bmatrix} & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & I_{n_{\xi+1}} \end{array}\right];$$

recall that $n_{\xi+1} = n - \operatorname{rank}(A)$. Then

$$\begin{aligned} \Pi_U^{\mathsf{T}} (\underbrace{S_U^* U^* A V S_V}_{\Sigma}) \Pi_V = \operatorname{diag}\Big(& \underbrace{\operatorname{diag}(\sigma_1 I_{\mu_1}, \sigma_2 I_{\mu_2}, \ldots, \sigma_\xi I_{\mu_\xi}, 0_{\mu_{\xi+1},0})}_{A_{11}}, \\ & \underbrace{\operatorname{diag}(\sigma_1 I_{m_1-\mu_1}, \sigma_2 I_{m_2-\mu_2}, \ldots, \sigma_\xi I_{m_\xi-\mu_\xi}, 0_{m_{\xi+1}-\mu_{\xi+1},n_{\xi+1}})}_{A_{22}} \Big) \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \end{aligned} \tag{4.25}$$

is the required block form.

4.3. Summary of the transformation

Let us briefly summarize the steps of the core problem revealing transformation:

$$\begin{aligned} A \times_1 \mathcal{X} &\approx \mathcal{B} && \text{(see (4.1))}, \\ A \times_1 [\![\mathcal{X} \,|\, I_n, R_2^*, \ldots, R_k^*]\!] &\approx [\![\mathcal{B} \,|\, I_m, R_2^*, \ldots, R_k^*]\!] && \text{(see (4.8))}, \\ (\underbrace{U^* A V}_{\Sigma}) \times_1 [\![\mathcal{X} \,|\, V^*, R_2^*, \ldots, R_k^*]\!] &\approx [\![\mathcal{B} \,|\, U^*, R_2^*, \ldots, R_k^*]\!] && \text{(see (4.14))}, \\ (S_U^* \overbrace{\Sigma} S_V) \times_1 [\![\mathcal{X} \,|\, S_V^* V^*, R_2^*, \ldots, R_k^*]\!] &\approx [\![\mathcal{B} \,|\, S_U^* U^*, R_2^*, \ldots, R_k^*]\!] && \text{(see (4.20))}, \\ (\Pi_U^{\mathsf{T}} \Sigma \Pi_V) \times_1 [\![\mathcal{X} \,|\, \Pi_V^{\mathsf{T}} S_V^* V^*, R_2^*, \ldots, R_k^*]\!] &\approx [\![\mathcal{B} \,|\, \Pi_U^{\mathsf{T}} S_U^* U^*, R_2^*, \ldots, R_k^*]\!] && \text{(see (4.25))}. \end{aligned}$$

Consequently, the original problem (4.1) is transformed by the unitary transformation (4.4) into a problem

$$\overbrace{\Big((\underbrace{U S_U \Pi_U}_{P})^* A (\underbrace{V S_V \Pi_V}_{Q}) \Big)}^{\widehat{A}} \times_1 \overbrace{[\![\mathcal{X} \,|\, Q^*, R_2^*, \ldots, R_k^*]\!]}^{\widehat{\mathcal{X}}} \approx \overbrace{[\![\mathcal{B} \,|\, P^*, R_2^*, \ldots, R_k^*]\!]}^{\widehat{\mathcal{B}}}, \tag{4.26}$$

where $R_j = [R_j', R_j'']$ are unitary matrices containing the left singular vectors of matricizations $\mathcal{B}^{\{j\}}$, $j = 2, \ldots, k$, i.e., from the Tucker decomposition of $\mathcal{B}$ (see (4.7)–(4.10)); U, V are unitary matrices containing the left and right singular vectors of A (see (4.11)–(4.13)); S_U, S_V are direct sums of unitary matrices containing the left singular vectors of F_ℓ matrices (see (4.19)–(4.18)); and Π_U, Π_V are permutations revealing the block structure.

The transformed system has the following system matrix

$$\widehat{A} = \left(\Pi_U^{\mathsf{T}}(\underbrace{S_U^* U^* A V S_V}_{\Sigma})\Pi_V\right) \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \tag{4.27}$$

where $A_{11} \in \mathbb{R}^{\mu \times \nu}$, $\mu \equiv \sum_{\ell=1}^{\xi+1} \mu_\ell$, $\nu \equiv \mu - \mu_{\xi+1})$, $A_{22} \in \mathbb{R}^{(m-\mu)\times(n-\nu)}$ are defined by (4.25). The tensor right-hand side is

$$\widehat{\mathcal{B}} = \mathrm{diag}_k(\mathcal{B}_1, 0), \quad \text{where} \quad \mathcal{B}_1 = [\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_\xi, \mathcal{H}_{\xi+1}]_1 \in \mathbb{F}^{\mu \times \delta_2 \times \cdots \times \delta_k}, \tag{4.28}$$

i.e., $\mathcal{B}_1$ is the concatenation of the tensors $\mathcal{H}_\ell$ (see (4.23)) along 1-mode fibers. The following definition formally introduces the tensor core problem.

Definition 4.3 *(Tensor core problem (TCP)).* The subproblem

$$A_{11} \times_1 \mathcal{X}_{1,1,\ldots,1} \approx \mathcal{B}_1$$

(see (4.6)) is called the tensor core problem (TCP) within a linear approximation problem $A \times_1 \mathcal{X} \approx \mathcal{B}$ (see (4.1)), if A_{11} and $\mathcal{B}_1$ are minimally dimensioned (and A_{22} maximally dimensioned) subject to the unitary transformation

$$[\![\mathcal{B} \,|\, P^*, R_2^*, \ldots, R_k^*]\!] \equiv \mathrm{diag}_k(\mathcal{B}_1, 0), \quad P^* A Q \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix},$$

where $P^* = P^{-1}$, $Q^* = Q^{-1}$, $R_j^* = R_j^{-1}$, $j = 2, \ldots, k$; cf. (4.5).

The above described construction gives a tensor subproblem having the following properties:

(CP1) The matrix A_{11} is of *full column rank*.

(CP2) The j-mode matricization $\mathcal{B}_1^{\{j\}}$ is of *full row rank*, or equivalently, all j-mode co-fibers of $\mathcal{B}$ are linearly independent, $j = 2, \ldots, k$.

(CP3) Let A_{11} have ξ distinct nonzero singular values with multiplicities μ_i and $\mu_{\xi+1} \equiv \dim(\mathcal{N}(A_{11}^*))$, and let U_i be matrices having orthonormal bases of left singular vector subspaces of A_{11} as their columns.
Then the matrices $U_i^* \mathcal{B}_1^{\{1\}}$ are of *full row rank* μ_i, for $i = 1, \ldots, \xi, \xi + 1$.

The following theorem states that the subproblem obtained by the construction above represents the core problem. We give the theorem without a proof since it can be derived fully analogously to the proof for the matrix right-hand side case in [9, Sect. 4.1, pp. 926–929], based on the properties (CP1)–(CP3).

Theorem 4.4 *(TCP revealing transformation). The unitary transformation developed in section 4.2 and summarized in (4.26)–(4.28) is the core problem revealing transformation, i.e., the system matrix* $A_{11} \in \mathbb{R}^{\mu\times\nu}$ *and the right-hand side tensor* $\mathcal{B}_1 \in \mathbb{F}^{\mu\times\delta_2\times\cdots\times\delta_k}$ *form the core problem*

$$A_{11} \times_1 \mathcal{X}_{1,1,\ldots,1} \approx \mathcal{B}_1$$

within $A \times_1 \mathcal{X} \approx \mathcal{B}$*. For an arbitrary unitary transformation of the form (4.5), yielding the same block structure with* $\widetilde{A}_{11} \in \mathbb{F}^{\widetilde{\mu}\times\widetilde{\nu}}$ *and* $\widetilde{\mathcal{B}}_1 \in \mathbb{F}^{\widetilde{\mu}\times\widetilde{\delta}_2\times\cdots\times\widetilde{\delta}_k}$*, it holds that*

$$\mu \le \widetilde{\mu}, \qquad \nu \le \widetilde{\nu}, \qquad \delta_j \le \widetilde{\delta}_j, \qquad j = 2,\ldots,k.$$

Note that the above obtained tensor core problem generalizes the *SVD form* of the matrix core problem; see [9].

5. Coupled TLS problems with tensor right-hand sides

The vector, or matrix, or tensor right-hand side TLS problem, and also the concept of the core problem within can be in the fully analogous way extended also to a set of coupled linear approximation problems

$$A \times_1 \mathcal{X}^{(t)} \approx \mathcal{B}^{(t)}, \quad \text{where} \quad t = 1,2,\ldots,\tau \tag{5.1}$$

and $A \in \mathbb{F}^{m\times n}$, $\mathcal{X}^{(t)} \in \mathbb{F}^{n\times d_2^{(t)}\times\cdots\times d_{k_t}^{(t)}}$, $\mathcal{B}^{(t)} \in \mathbb{F}^{m\times d_2^{(t)}\times\cdots\times d_{k_t}^{(t)}}$. The right-hand side tensors of each of these problems may be of *different orders* (including the second and the first order tensors, i.e., matrices and vectors, respectively), and *different dimensions* except for the first one. Therefore, neither the right-hand sides $\mathcal{B}^{(t)}$ nor the solutions $\mathcal{X}^{(t)}$ can be concatenated into one big tensor, in general.

Definition 5.1 *(Coupled TLS problems).* Let $A \times_1 \mathcal{X}^{(t)} \approx \mathcal{B}^{(t)}$, $t = 1,2,\ldots,\tau$ be the set of approximation problems (5.1). The minimization problem

$$\min_{\substack{\mathcal{G}^{(1)} \in \mathbb{F}^{m\times d_2^{(1)}\times\cdots\times d_{k_1}^{(1)}} \\ \vdots \\ \mathcal{G}^{(\tau)} \in \mathbb{F}^{m\times d_2^{(\tau)}\times\cdots\times d_{k_\tau}^{(\tau)}} \\ E \in \mathbb{F}^{m\times n}}} \left(\left(\sum_{t=1}^{\tau} \|\mathcal{G}^{(t)}\|^2 \right) + \|E\|_F^2 \right)^{\frac{1}{2}} \quad \text{subject to} \tag{5.2}$$

$$(A + E) \times_1 \mathcal{X}^{(t)} = \mathcal{B}^{(t)} + \mathcal{G}^{(t)}, \qquad t = 1,2,\ldots,\tau$$

is called the coupled TLS problem.

Employing the matricizations of all the right-hand sides, the coupled problem can be rearranged while putting everything together into one big matrix problem

$$A\Big[(\mathcal{X}^{(1)})^{\{1\}}, (\mathcal{X}^{(2)})^{\{1\}}, \dots, (\mathcal{X}^{(\tau)})^{\{1\}}\Big] \approx \Big[(\mathcal{B}^{(1)})^{\{1\}}, (\mathcal{B}^{(2)})^{\{1\}}, \dots, (\mathcal{B}^{(\tau)})^{\{1\}}\Big]. \qquad (5.3)$$

Note that each block $(\mathcal{B}^{(t)})^{\{1\}}$ may have a *different number of columns*. Then the solution of the coupled problem can be found in the same way as shown in section 4.1; see in particular Theorem 4.2. The concept of the core problem can be introduced analogously; cf. Definition 4.3.

Definition 5.2 *(Coupled core problem).* The set of subproblems

$$A_{11} \times_1 \mathcal{X}^{(t)}_{1,1,\dots,1} \approx \mathcal{B}^{(t)}_1, \qquad t = 1, 2, \dots, \tau,$$

is called the coupled core problem within (5.1) if A_{11} and $\mathcal{B}^{(t)}_1$ are minimally dimensioned (and A_{22} maximally dimensioned) subject to the unitary transformations

$$[\![\mathcal{B}^{(t)} \,|\, P^*, (R^{(t)}_2)^*, \dots, (R^{(t)}_{k_t})^*]\!] \equiv \mathrm{diag}_{k_t}(\mathcal{B}^{(t)}_1, 0), \quad P^* A Q \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix}, \qquad (5.4)$$

where $P^* = P^{-1}$, $Q^* = Q^{-1}$, $(R^{(t)}_j)^* = (R^{(t)}_j)^{-1}$, $j = 2, \dots, k_t$, $t = 1, 2, \dots, \tau$. (Note that P and Q are independent on t.)

The construction described in sections 4.2.1–4.2.4 can also be generalized to coupled TLS problems. We start with the Tucker decomposition of all right-hand side tensors while forming the tensors $\mathcal{C}^{(t)}$ as in (4.10). Then, using the SVD of A we get right-hand sides $\mathcal{F}^{(t)}$ as in (4.15). Partitioning of

$$\Big[(\mathcal{F}^{(1)})^{\{1\}}, (\mathcal{F}^{(2)})^{\{1\}}, \dots, (\mathcal{F}^{(\tau)})^{\{1\}}\Big]$$

to block-rows with vertical dimensions given by the multiplicities of the singular values of A and the dimension of the null-space of A^* (see (4.17) and Fig. 3), with the subsequent SVDs of these blocks (see (4.18)) allows us to assemble the S_U and S_V matrices in the same way as in (4.19). The final permutation (see section 4.2.4) reveals the block structure (5.4) simultaneously, i.e., for all $t = 1, 2, \dots, \tau$ at the same time. Such construction yields the set of subproblems, which has the minimality property mentioned above, and therefore represents the coupled core problem.

6. Discussion and comparison of the results

It is particularly interesting to compare the results of sections 4.2 and 4.3 with those obtained previously for the matrix right-hand side problems in the view of the relation given in section 4.1 (see Theorem 4.2). The TLS problem with the tensor right-hand side

$$A \times_1 \mathcal{X} \approx \mathcal{B} \qquad \text{can always be matricized as} \qquad A\mathcal{X}^{\{1\}} \approx \mathcal{B}^{\{1\}}, \qquad (6.1)$$

and instead of the tensor minimization (4.2) the matrix minimization (2.9) can be considered. Theorem 4.2 says that both approaches yield mathematically the same minima and the same TLS solution(s), up to the 1-mode matricization.

The core problem point of view, however, reveals some differences. Let

$$[\![\mathcal{B} \,|\, P^*, R_2^*, \ldots, R_k^*]\!] \equiv \operatorname{diag}_k(\mathcal{B}_1, 0), \qquad P^* A Q \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \tag{6.2}$$

be the *tensor core problem* within $A \times_1 \mathcal{X} \approx \mathcal{B}$, and

$$\widetilde{P}^* \mathcal{B}^{\{1\}} R \equiv \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}, \qquad \widetilde{P}^* A \widetilde{Q} \equiv \begin{bmatrix} \widetilde{A}_{11} & 0 \\ 0 & \widetilde{A}_{22} \end{bmatrix} \tag{6.3}$$

the *matrix core problem* (see section 2.2) within the matricized problem $A\mathcal{X}^{\{1\}} \approx \mathcal{B}^{\{1\}}$. Since the (same) SVD of A, $A = U\Sigma V^*$ appears in both core problem revealing transformations and the projections of the 1-mode fibers of $\mathcal{B}$ and the columns of $\mathcal{B}^{\{1\}}$ onto the left singular vector spaces of A are the same, the only important difference appears in the right-hand side preprocessing.

Recall that 1-mode fibers of $\mathcal{F}$ (see (4.15)) represent linear combinations of the columns of the above mentioned projections $U^* \mathcal{B}^{\{1\}}$. The number of linearly independent 1-mode co-fibers of its subtensors $\mathcal{F}_\ell$ (see (4.17)) is clearly the same as the number of the linearly independent rows of $F_\ell = \mathcal{F}_\ell^{\{1\}}$. Therefore, the choice of S_ℓ (see (4.18)–(4.21)) is independent on the choice of the unitary matrices R_j performing the linear combinations of 1-mode-fibers of $\mathcal{B}$ in j-modes, $j = 2, \ldots, k$ (see (4.15)), and on the unitary matrix R performing combinations of columns of $U^* \mathcal{B}^{\{1\}}$ in revealing of (6.3). Thus, the matrices S_U, S_V, the subsequent permutations Π_U, Π_V, and also the blocks A_{11}, A_{22} are in both transformations (6.2) and (6.3) the same, i.e., in particular $A_{11} = \widetilde{A}_{11}$ and $A_{22} = \widetilde{A}_{22}$. Consequently, also the length of 1-mode fibers of $\mathcal{B}_1$ equals to the number of rows of B_1. Thus, in general, the most important difference (originated in the preprocessing) is in the number of individual right-hand sides. In particular, the number of 1-mode fibers of $\mathcal{B}_1$ (i.e., the number of columns of $\mathcal{B}_1^{\{1\}}$) may differ from the number of columns of B_1. Clearly, the right-hand sides satisfy

$$\mathcal{B}_1^{\{1\}} \left(\overline{R_k'} \otimes \cdots \otimes \overline{R_2'} \right)^* = [B_1, 0] R^*.$$

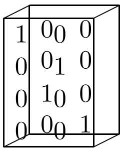
Consequently, both core problems are the same (after reshaping the tensor by the 1-mode matricization) *if and only if*

$$\overline{R_k} \otimes \cdots \otimes \overline{R_2} = R \in \mathbb{F}^{d \times d}, \qquad \text{where} \qquad d \equiv \textstyle\prod_{j=2}^{k} d_j, \tag{6.4}$$

i.e., if and only if the preprocessings of the right-hand sides of the two problems in (6.1) yield the same result. The following examples illustrate the situation where the core problems are equivalent (see Example 6.1) and different (see Example 6.2).

Example 6.1. Consider an approximation problem $A \times_1 \mathcal{X} \approx \mathcal{B}$, where $A \in \mathbb{R}^{4\times 3}$, $\operatorname{rank}(A) = 3$, and

$$\mathcal{B} =$$



$$, \quad \mathcal{B}^{\{1\}} = \left[\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right].$$

Since $\mathcal{B}^{\{1\}}$, $\mathcal{B}^{\{2\}}$, and $\mathcal{B}^{\{3\}}$ are of full row rank, $\mathcal{B}$ is the Tucker core by itself. The matricized problem $A\mathcal{X}^{\{1\}} \approx \mathcal{B}^{\{1\}}$ has full column rank right-hand side matrix $\mathcal{B}^{\{1\}}$. Therefore, the right-hand side preprocessing is not present in the tensor, as well as in the matrix core problem reduction. Let $A = U\Sigma V^{\mathsf{T}}$ be the SVD of A, i.e. $\Sigma \in \mathbb{R}^{4\times 3}$ and U, V are unitary matrices. Following the tensor reduction derived in the previous sections, we obtain

$$A_{11} \times_1 \mathcal{X}_{1,1,1} \approx \mathcal{B}_1, \quad A_{11} = \Sigma, \quad \mathcal{B}_1 = U^{\mathsf{T}} \times_1 \mathcal{B}, \quad \text{and} \quad R_2 = R_3 = I_2, \quad R_3 \otimes R_2 = I_4.$$

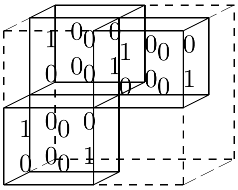
Applying the reduction to the so-called SVD form (see [9]), we get

$$A_{11}\mathcal{X}_1^{\{1\}} \approx \mathcal{B}_1^{\{1\}}, \quad A_{11} = \Sigma, \quad \mathcal{B}_1^{\{1\}} = U^{\mathsf{T}}\mathcal{B}^{\{1\}}, \quad \text{and} \quad R = I_4.$$

We see, that $R_3 \otimes R_2 = R$ and thus the core problem of the matricized problem is the matricized tensor core problem. This clearly implies that the approaches based on tensor core reduction and based on matricization lead to the same result.

Example 6.2. Consider an approximation problem $A \times_1 \mathcal{X} \approx \mathcal{B}$, where $A \in \mathbb{R}^{4\times 3}$, $\operatorname{rank}(A) = 3$, and

$$\mathcal{B} =$$



$$, \quad \mathcal{B}^{\{1\}} = \left[\begin{array}{cccc|cccc|cccc|cccc} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right].$$

Since the tensor is so-called super-symmetric, all three matricizations give the same matrix $\mathcal{B}^{\{1\}} = \mathcal{B}^{\{2\}} = \mathcal{B}^{\{3\}}$ of full row rank. Thus $\mathcal{B}$ again represent the Tucker core by itself. Let $A = U\Sigma V^{\mathsf{T}}$ be the SVD of A. Similarly as in Example 6.1, the tensor reduction gives

$$A_{11} \times_1 \mathcal{X}_{1,1,1} \approx \mathcal{B}_1, \quad A_{11} = \Sigma, \quad \mathcal{B}_1 = U^{\mathsf{T}} \times_1 \mathcal{B}, \quad \text{and} \quad R_2 = R_3 = I_4, \quad R_3 \otimes R_2 = I_{16}.$$

However, considering the approach based on matricization, the right-hand side $\mathcal{B}^{\{1\}}$ has to be preprocessed as follows

$$\mathcal{B}^{\{1\}} = \underbrace{\begin{bmatrix} 2^{\frac{1}{2}} & 0 & 0 & 0 \\ 0 & 2^{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{C} \underbrace{\left[\begin{array}{cccc|cccc|cccc|cccc} 0 & 0 & 2^{-\frac{1}{2}} & 0 & 0 & 0 & 0 & 0 & 2^{-\frac{1}{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2^{-\frac{1}{2}} & 0 & 0 & 0 & 0 & 0 & 2^{-\frac{1}{2}} & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]}_{(R')^{\mathsf{T}}}.$$

Consequently, the reduction to the SVD form gives

$$A_{11}\mathcal{X}_1^{\{1\}} \approx \mathcal{B}_1^{\{1\}}, \quad A_{11} = \Sigma, \quad \mathcal{B}_1^{\{1\}} = U^{\mathsf{T}}C, \quad \text{and} \quad R = [R', R''], \quad R^{-1} = R^{\mathsf{T}} \in \mathbb{R}^{16\times 16}.$$

From the pattern of (non)zero entries of R, it is visible that R cannot be written as a Kronecker product of two matrices of order four, i.e., $R_3 \otimes R_2 \neq R$. In summary, the approaches based on tensor core reduction and based on matricization are not equivalent here.

Recall that the core problem is unique up to a unitary transformation. Thus we are interested in the dimensions of the core problem and not necessarily in the particular entries of A_{11} and $\mathcal{B}_1$. The previous discussion implies the following corollary.

Corollary 6.3. *Let* $A \times_1 \mathcal{X} \approx \mathcal{B}$ *be a linear approximation problem with the tensor right-hand side and* $AX \approx B$, $X \equiv \mathcal{X}^{\{1\}}$, $B \equiv \mathcal{B}^{\{1\}}$ *its matricized counterpart. Let* $A_{11} \times_1 \mathcal{X}_1 \approx \mathcal{B}_1$ *and* $\widetilde{A}_{11}X_1 \approx B_1$ *be the core problems within the two formulations, where* P, Q, $R_2, \ldots, R_k$ *and* $\widetilde{P}$, $\widetilde{Q}$, R *are the unitary matrices of the respective core problem revealing transformations.*

Then A_{11} *and* $\widetilde{A}_{11}$ *are always of the same dimensions. However,* $\mathcal{B}^{\{1\}}$ *and* B_1 *are of the same dimensions if and only if the matrix* $\overline{R_k} \otimes \cdots \otimes \overline{R_2}$ *is a unitary transformation of the matrix* R.

In summary, for tensor right-hand side problems we can choose between two core approaches:

- keeping the tensor structure while revealing the tensor core problem, or
- matricization while revealing the matrix core problem.

The principal difference can also be illustrated in Fig. 3. In the matricized problem, the unitary transformation R performs linear combinations of all 1-mode fibers while preserving the Frobenius norm of the horizontal slices (in general 1-mode co-fibers). In the tensor setting, unitary transformations R_j, $j = 2, 3$, perform linear combinations of 1-mode fibers that belong only to frontal or lateral slices (in general $(1, j)$-mode slice), respectively, while preserving the Euclidean norm of j-mode fibers. We see that revealing the core problem while preserving the tensor structure is significantly more constrained. The condition (6.4) is in general rarely satisfied.

Analogously, the coupled core problem within (5.1) can be compared with its matrix counterpart within (5.3). The core problems are the same (after reshaping the tensor by the 1-mode matricization) *if and only if*

$$\operatorname{diag}\left(\overline{R_{k_1}^{(1)}} \otimes \cdots \otimes \overline{R_2^{(1)}}, \overline{R_{k_2}^{(2)}} \otimes \cdots \otimes \overline{R_2^{(2)}}, \ldots, \overline{R_{k_\tau}^{(\tau)}} \otimes \cdots \otimes \overline{R_2^{(\tau)}}\right) = R \in \mathbb{F}^{d \times d}, \qquad (6.5)$$

$$\text{where} \qquad d \equiv \textstyle\sum_{t=1}^{\tau} \prod_{j=2}^{k_t} d_j^{(t)}.$$

Consequently, a corollary analogous to Corollary 6.3 can be formulated also for the coupled problem.

In general, the application of the core problem reduction on a problem with highly structured right-hand side *restricts* the possibilities for choosing the unitary matrix R. In both cases above we require R to belong into some *subgroup* of the whole unitary group $\mathbb{U}(d)$ of degree d.

Recall that the core problem within the matrix (multiple) right-hand side approximation problem (see section 2.2) may not have a TLS solution, contrary to the vector (single) right-hand side case. The possible nonexistence of the TLS solution is closely related to the structure of the right-hand side as it has been recently shown in [6]. We see, that further increasing the order of the right-hand side tensor from a matrix (i.e., two-way tensor) to a general k-way tensor does not change the behavior of the TLS formulation from the solvability point of view. It involves only the size of the core problem within.

7. Conclusions

We have introduced the definition of the TLS problem within approximation problems with (single or multiple) tensor right-hand sides allowing to apply directly the results on the existence and uniqueness of the TLS solution available for the standard matrix right-hand side problems. We have proved that, on the other hand, the necessary and sufficient information for solving the tensor right-hand side problem and its matricized counterpart can be different. We have shown that there exists the minimally dimensioned core problem within the TLS problem with a tensor right-hand side, by deriving the core reduction transformation. The tensor core problem is, in general, larger than the core problem within the matricized problem, since it respects the structure given by the multiway configuration of the original tensor right hand-side. This work represents the first step towards investigation of fully tensorized (general or structured) linear approximation problems of the form $\mathcal{A} \times_{\ldots} \mathcal{X} \approx \mathcal{B}$, where all $\mathcal{A}$, $\mathcal{X}$, and $\mathcal{B}$ are tensors of higher orders and "$\times_{\ldots}$" a tensor-tensor product in appropriate modes. Since the tensor formulation covers also the formulations analyzed previously, we believe the results can be used in further analysis of single and multiple right-hand side TLS problems.

Acknowledgements

The authors wish to thank the anonymous referee for her or his useful comments.

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Linear Algebra and its Applications 577 (2019) 1–20

Contents lists available at ScienceDirect

Linear Algebra and its Applications

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On TLS formulation and core reduction for data fitting with generalized models ☆

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A R T I C L E I N F O

Article history:
Received 28 June 2018
Accepted 12 April 2019
Available online 16 April 2019
Submitted by H. Fassbender

MSC:
15A09
15A21
15A69
65F20
65F25

Keywords:
Total least squares problem (TLS)
Error-in-variables modeling
Orthogonal regression
Multiple observations
Core problem
Tensor approximation problem

A B S T R A C T

The total least squares (TLS) framework represents a popular data fitting approach for solving matrix approximation problems of the form $\mathcal{A}(X) \equiv AX \approx B$. A general linear mapping on spaces of matrices $\mathcal{A} : X \longmapsto B$ can be represented by a fourth-order tensor which is in the $AX \approx B$ case highly structured. This has a direct impact on solvability of the corresponding TLS problem, which is known to be complicated. Thus this paper focuses on several generalizations of the model $\mathcal{A}$: the bilinear model, the model of higher Kronecker rank, and the fully tensorized model. It is shown how the corresponding generalization of the TLS formulation induces enrichment of the search space for the data corrections. Solvability of the resulting minimization problem is studied. Furthermore, extension of the so-called core reduction to the bilinear model is presented. For the fully tensor model, its relation to a particular single right-hand side TLS problem is derived. Relationships among individual formulations are discussed.

☆ This work has been partially supported by the SGS grant of Technical University of Liberec No. SGS-2019-4037, and by the GACR grant No. 17-04150J.

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https://doi.org/10.1016/j.laa.2019.04.018

1. Introduction

One of the typical tasks arising in the area of data fitting is the solution of linear approximation problems with a matrix model and a matrix (or so-called multiple) right-hand side,

$$AX \approx B, \quad A \in \mathbb{F}^{m\times n}, \quad B \in \mathbb{F}^{m\times d}, \tag{1.1}$$

where $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$. When the errors are present both in the model A and the observations B, the *total least squares* (TLS) method is preferred, which however yields several principal difficulties (see [23], [26], [27], [28], [6], [5]). In particular, the TLS problem *may not have a solution* or the solution may not be unique; see [2] for the (so-called single right-hand side) case $d = 1$ and [28], [5], [9] for the general case. The *core reduction* developed in [18] for $d = 1$ and in [7], [8], [4] for $d \geq 1$, allows to extract the necessary and sufficient data from A, B by employing a specific unitary transformation on the original problem. This approach does not (except of reducing the dimensions of the problem) necessarily simplify the solvability of the approximation problem, since the resulting (typically small dimensional) core problem still may not have a solution. The existence of the (unique) TLS solution is ensured only in the single right-hand side case, i.e., when $d = 1$. Moreover, such solution (for $d = 1$) can be unitarily transformed back to obtain the (minimum norm) TLS solution of the original problem if it exists, or the so-called (minimum norm) nongeneric solution (otherwise); see [18].

The right-hand side matrix B arises essentially in two different ways. Either the columns of B represent d individual observations (for example when the observation depends on a parameter that can be sampled), or B is a single observation of the matrix form; see, e.g., [21], [22] for particular applications. If the observation depends on several parameters, their sampling leads to a set of observations forming a structured (typically tensor) right-hand side. A TLS formulation and core reduction for such problems have been proposed and analyzed recently in [10]. In this paper, we consider the observation to be a matrix and concentrate on the model setting.

The fundamental difficulty of TLS (not present in other formulations such as ordinary LS) is possible nonexistence of the solution. Situations where this happens were fully classified in the paper [5] revealing that the problem lies in the fact that the search set for the corrections of the data B, A is too limited. To see this, note that in (1.1) our goal is in fact to find a single matrix pre-image X of the single matrix observation B. Generally, X and B could be linked through a linear model $\mathcal{A}(X) \approx B$, where $\mathcal{A}$ is a general linear mapping from a space of matrices to another space of matrices. Thus $\mathcal{A}$ can be represented by a four-way array, i.e., a *fourth-order tensor*. The problem (1.1) is then just a special case of this setting. Since the model is here represented by a single matrix A, TLS framework allows only matrix corrections of both A and B.

In this paper we try to better understand the above described limitations, in particular in the context of the core problem theory. We consider several generalizations of the setting of the original model such that defining a natural generalization of the TLS minimization for the related approximation problem results in *enrichment of the search space* for the model corrections. First, we analyze a *bilinear model* appearing in various applications (see [13], [14]) and the corresponding TLS minimization. We derive the core reduction for the bilinear model, which is the main result of this paper. Further, the extension to a *higher Kronecker rank model* (i.e., sum of bilinear models) is noted. Recall that models of the Kronecker rank two appear, e.g., in connection with Sylvester or Lyapunov equations, etc. Then, approximation problems with a *fully tensorized model* are considered. Here we show that the search set is so rich that the approximation problem can be transformed (through vectorization) into a single right-hand side approximation problem. This allows to apply the core reduction available for single right-hand side problems directly, and therefore simplify the solvability classification. Relationships among individual generalizations are discussed.

In general, we consider a linear mapping $\mathcal{A} : \mathscr{U} \longrightarrow \mathscr{V}$ between finite-dimensional linear vector spaces $\mathscr{U}$ and $\mathscr{V}$ over the same field $\mathbb{F}$, i.e., $\mathcal{A} \in \mathscr{L}(\mathscr{U}, \mathscr{V})$ being the set of all such mappings, with the range $\mathscr{R}(\mathcal{A}) \subsetneq \mathscr{V}$. The *linear approximation problem*

$$\mathcal{A}(x) \approx b, \qquad \text{where} \qquad b \in \mathscr{V} \quad \text{but} \quad b \notin \mathscr{R}(\mathcal{A}) \tag{1.2}$$

is replaced by the TLS minimization

$$\min_{\substack{g \in \mathscr{V} \\ \mathcal{E} \in \mathscr{E} \subseteq \mathscr{L}(\mathscr{U}, \mathscr{V})}} \quad \|(g, \mathcal{E})\|_{\star} \qquad \text{subject to} \qquad (\mathcal{A} + \mathcal{E})(x) = b + g, \tag{1.3}$$

where $\mathcal{E}$, the correction of our model is taken from some *search set* $\mathscr{E}$, that may be in general a subspace or submanifold of $\mathscr{L}(\mathscr{U}, \mathscr{V})$. Here $\|\cdot\|_{\star}$ denotes some norm in $\mathscr{V} \times \mathscr{L}(\mathscr{U}, \mathscr{V})$. We consider the Euclidean and Frobenius norms of vectors and matrices, respectively, and their natural extension to tensors. However, any general unitarily invariant norm (see [19, Chap. II.3], [25], [15], [24]) can be considered for the (unitary) core problem transformation and subsequent reduction.

This paper is organized as follows. Section 2 recapitulates TLS formulations for problems with a matrix model and various objects (vectors, matrices, and tensors) on the right-hand side. Section 3 is the key part introducing and analyzing problems with various generalizations of the model setting. Section 4 concludes the paper.

Throughout the paper I_ℓ (or just I) denotes an $\ell \times \ell$ identity matrix and $e_i^{(\ell)}$ (or just e_i) its ith column; $0_{\ell,\xi}$ (or just 0) denotes an $\ell \times \xi$ zero matrix; and M^{T}, $M^* \equiv \overline{M}^{\mathsf{T}}$, $\mathscr{R}(M)$, and $\mathscr{N}(M)$ denote the transposition, the Hermitian conjugation, the range, and the null-space of a matrix M, respectively. Further, $M \otimes K$ denotes the Kronecker product of matrices where $m_{i,j}$, the (i,j)th entry of M is replaced by the block $m_{i,j}K$. For a tensor $\mathcal{T} \in \mathbb{F}^{n_1 \times n_2 \times \cdots \times n_k}$, we consider three types of subarrays:

- n/n_p subarrays in $\mathbb{F}^{1\times\cdots\times 1\times n_p\times 1\times\cdots\times 1}$ called the *p-mode fibers*, trivially isomorphic with vectors of length n_p (the fibers of a two-way tensor are called the columns and rows);
- $n/(n_p n_u)$ subarrays in $\mathbb{F}^{1\times\cdots\times 1\times n_p\times 1\times\cdots\times 1\times n_u\times 1\times\cdots\times 1}$ called the *(p,u)-modes slices*, trivially isomorphic with n_p-by-n_u matrices (the slices of a three-way tensor are called frontal, lateral, and horizontal);
- n_p subarrays in $\mathbb{F}^{n_1\times\cdots\times n_{p-1}\times 1\times n_{p+1}\times\cdots\times n_k}$ called the *p-mode co-fibers*, trivially isomorphic with $(k-1)$-way tensors.

Note that arranging of all the p-mode fibers into one matrix $\mathcal{T}^{\{p\}} \in \mathbb{F}^{n_p\times((\prod_{j=1}^{k} n_j)/n_p)}$ in a lexicographical order w.r.t. multiindices $(i_k,\ldots,i_{p+1},i_{p-1},\ldots,i_1)$ is called the *p-mode matricization* of tensor $\mathcal{T}$; see, e.g., [12], [20, Chap. 3.1.2].

2. Preliminaries

In the classical setting, the mapping $\mathcal{A}$ is represented by a single matrix A called the *system (or model) matrix*. The structure of the right-hand side depends on the number of observations being available for this model, and, in particular, on the number of free parameters involving the observations. Now we summarize basic TLS formulations and the corresponding core theory studied previously.

2.1. TLS formulations for various right-hand sides

In the simplest case of (1.2), we have just *one observation* forming an m-vector. The so-called *single (or vector) right-hand side* problem then takes the form

$$Ax \approx b, \quad \text{where} \quad A \in \mathbb{F}^{m\times n}, \quad x \in \mathbb{F}^{n}, \quad b \in \mathbb{F}^{m}. \tag{2.1}$$

If the observation depends, e.g., on *one free parameter*, considering d samples of its value, we obtain d vectors forming a matrix. This so-called *multiple (or matrix) right-hand side problem* takes the form

$$AX \approx B, \quad \text{where} \quad A \in \mathbb{F}^{m\times n}, \quad X \in \mathbb{F}^{n\times d}, \quad B \in \mathbb{F}^{m\times d}. \tag{2.2}$$

In the case of $(k-1)$ *free parameters*, having d_{j+1} samples of the value of the jth parameter, observations made on a full Cartesian grid of sampled parameters form a k-way tensor. This *tensor right-hand side problem* takes the form

$$A \times_1 \mathcal{X} \approx \mathcal{B}, \quad \text{where} \quad A \in \mathbb{F}^{m\times n}, \quad \mathcal{X} \in \mathbb{F}^{n\times d_2\times\cdots\times d_k}, \quad \mathcal{B} \in \mathbb{F}^{m\times d_2\times\cdots\times d_k}. \tag{2.3}$$

Here $\mathcal{S} = M \times_\ell \mathcal{T}$ denotes the *ℓ-mode matrix-tensor product.*[1] In other words, the ℓ-mode fibers of the tensor $\mathcal{S}$ are obtained as matrix-vector products of the matrix M with ℓ-mode fibers of $\mathcal{T}$, where the fibers are handled as column vectors; see, e.g., [1], [20].

The respective TLS minimizations (1.3) are considered as:

$$\min_{E \in \mathbb{F}^{m\times n},\, g \in \mathbb{F}^{m}} \|[g, E]\|_F \quad \text{subject to} \quad (A+E)x = b+g, \tag{2.4}$$

$$\min_{E \in \mathbb{F}^{m\times n},\, G \in \mathbb{F}^{m\times d}} \|[G, E]\|_F \quad \text{subject to} \quad (A+E)X = B+G, \tag{2.5}$$

$$\min_{E \in \mathbb{F}^{m\times n},\, \mathcal{G} \in \mathbb{F}^{m\times d_2\times\cdots\times d_k}} (\|E\|_F^2 + \|\mathcal{G}\|^2)^{\frac{1}{2}} \quad \text{subject to} \quad (A+E)\times_1 \mathcal{X} = \mathcal{B}+\mathcal{G}. \tag{2.6}$$

Here the norm $\|\mathcal{T}\|$ of a tensor $\mathcal{T}$ is the natural extension of the Euclidean and Frobenius norms of a column vector and a matrix, respectively, i.e., $\|\mathcal{T}\|$ is the square-root of sum of squares of entries of $\mathcal{T}$; see [12]. We call it simply the *tensor norm*.

Note that if the observations in (2.3) are not available for the full Cartesian grid, it is possible to reformulate the approximation problem as a set of coupled TLS problems with several differently structured right-hand sides and the same matrix; for more details see [10].

2.2. The core problem transformation

Based on the unitary invariance of the Euclidean, Frobenius, and tensor norms, the so-called *core problem* theory was developed for the vector right-hand sides problems (2.4) in the works [16], [17], [18]; for the matrix right-hand sides problems (2.5) in [7], [8], and [4]; and for the tensor right-hand sides problems (2.6) in [10]. It was shown that in these three respective cases there exist: A pair of unitary matrices $P \in \mathbb{F}^{m\times m}$, $Q \in \mathbb{F}^{n\times n}$; a triplet of unitary matrices $P \in \mathbb{F}^{m\times m}$, $Q \in \mathbb{F}^{n\times n}$, $R \in \mathbb{F}^{d\times d}$; and a $(k+1)$tuple of unitary matrices $P \in \mathbb{F}^{m\times m}$, $Q \in \mathbb{F}^{n\times n}$, $R_j \in \mathbb{F}^{d_j\times d_j}$, $j = 2, \ldots, k$, so that

$$[\widehat{b}\,|\,\widehat{A}] = P^*[b\,|\,A]\begin{bmatrix} 1 & 0 \\ 0 & Q \end{bmatrix} \equiv \left[\begin{array}{c|cc} b_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{array}\right]; \tag{2.7}$$

$$[\widehat{B}\,|\,\widehat{A}] = P^*[B\,|\,A]\begin{bmatrix} R & 0 \\ 0 & Q \end{bmatrix} \equiv \left[\begin{array}{cc|cc} B_1 & 0 & A_{11} & 0 \\ 0 & 0 & 0 & A_{22} \end{array}\right]; \tag{2.8}$$

and

---

[1] In the literature, this product is usually defined in the opposite order (as the tensor-matrix product $\mathcal{X} \times_1 A$). We deviate here from this convention in order to stay notationally consistent through the formulations of linear approximation problems in (2.1)–(2.3).

$$\begin{aligned} \widehat{\mathcal{B}} = R_k^* \times_k (\cdots \times_3 (R_2^* \times_2 (P^* \times_1 \mathcal{B}))\cdots) \equiv \mathrm{diag}_k(\mathcal{B}_1, 0), \\ \widehat{A} = P^* A Q \equiv \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix}, \end{aligned} \tag{2.9}$$

where $\mathrm{diag}_k(\cdots)$ forms a k-way block diagonal tensor, a direct sum of its k-way tensor arguments. Corresponding transformations of the unknown objects,

$$\widehat{x} = Q^* x, \qquad \widehat{X} = Q^* X R, \qquad \widehat{\mathcal{X}} = R_k^* \times_k (\cdots \times_3 (R_2^* \times_2 (P^* \times_1 \mathcal{X}))\cdots),$$

together with conformal partitionings

$$\widehat{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \qquad \widehat{X} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}, \qquad \widehat{\mathcal{X}} = [\mathcal{X}_{i_1,i_2,\ldots,i_k}],\ i_j = 1,2,\ j = 1,2,\ldots,k, \tag{2.10}$$

separate the original problems (2.1)–(2.3) into two, four, and 2^k independent subproblems, respectively. Then

$$A_{11} x_1 \approx b_1, \qquad A_{22} x_2 \approx 0; \tag{2.11}$$

$$A_{11} X_{11} \approx B_1, \qquad A_{11} X_{12} \approx 0, \qquad A_{22} X_{21} \approx 0, \qquad A_{22} X_{22} \approx 0; \tag{2.12}$$

and

$$\begin{aligned} A_{11} \times_1 \mathcal{X}_{1,1,\ldots,1} \approx \mathcal{B}_1, \quad A_{11} \times_1 \mathcal{X}_{1,i_2,\ldots,i_k} \approx 0, \quad A_{22} \times_1 \mathcal{X}_{2,1,\ldots,1} \approx 0, \\ A_{22} \times_1 \mathcal{X}_{2,i_2,\ldots,i_k} \approx 0, \end{aligned} \tag{2.13}$$

where $(i_2, \ldots, i_k) \in \{1,2\}^{k-1}$ but $(i_2, \ldots, i_k) \neq (1, \ldots, 1)$. Clearly, in all three cases only the first problem needs to be solved, all the other have zero solutions.

Moreover, the unitary matrices P, Q, R, R_j, $j = 2, \ldots, k$, can always be chosen in such a way that:

(CP1) The matrix $A_{11} \in \mathbb{F}^{\mu \times \nu}$ is of *full column rank* ν.
(CP2) The vector $b_1 \in \mathbb{F}^{\mu}$ is *nonzero.*

- The matrix $B_1 \in \mathbb{F}^{\mu \times \delta}$ is of *full column rank* δ.
- The tensor $\mathcal{B}_1 \in \mathbb{F}^{\mu \times \delta_2 \times \cdots \times \delta_k}$ has j-mode matricizations $\mathcal{B}_1^{\{j\}}$ of *full row rank* δ_j (or equivalently, all j-mode co-fibers of $\mathcal{B}_1$ are linearly independent), for $j = 2, \ldots, k$.

Let A_{11} have ξ distinct nonzero singular values with multiplicities μ_i and $\mu_{\xi+1} \equiv \dim(\mathcal{N}(A_{11}^*))$, and let U_i be matrices having orthonormal bases of left singular vector subspaces of A_{11} as their columns. Then:

(CP3) The $\mu_1 = \ldots = \mu_\xi = \mu_{\xi+1} = 1$ and $U_i^* b_1 \in \mathbb{F}$ are *nonzero*, for $i = 1, \ldots, \xi, \xi + 1$.

- The matrices $U_i^* B_1 \in \mathbb{F}^{\mu_i \times \delta}$ are of *full row rank* μ_i, for $i = 1, \ldots, \xi, \xi + 1$.
- The matrices $U_i^* \mathcal{B}_1^{\{1\}} \in \mathbb{F}^{\mu_i \times (\prod_{j=2}^{k} \delta_j)}$ are of *full row rank* μ_i, for $i = 1, \ldots, \xi, \xi + 1$.

The subproblems

$$A_{11}x_1 \approx b_1, \quad A_{11}X_{11} \approx B_1, \quad \text{and} \quad A_{11} \times_1 \mathcal{X}_{1,1,\ldots,1} \approx \mathcal{B}_1 \tag{2.14}$$

satisfying (CP1)–(CP3) are called the single (or vector), multiple (or matrix), and tensor right-hand side *core problem* within (2.1)–(2.3), respectively. The core problem is always given *uniquely* up to a unitary transformation, because such transformation does not change its fundamental properties (CP1)–(CP3). In other words, in the vector right-hand side case, the particular core problem matrix $[b_1, A_{11}]$ has to be seen only as a *representative* of the set of all possible matrices

$$\left\{ [\widetilde{b}_1, \widetilde{A}_{11}] \ : \ \widetilde{A}_{11} = P_1^* A_{11} Q_1, \quad \widetilde{b}_1 = P_1^* b_1, \quad P_1^* = P_1^{-1}, \quad Q_1^* = Q_1^{-1} \right\}$$

representing the same core problem. Similar result holds in the matrix and tensor right-hand side case.

Properties (CP1)–(CP3) imply a lot of important properties of core problems, in particular, the core problems are the smallest (in terms of dimensions) subproblems that can be obtained by unitary transformations giving the block partitionings of the form (2.7)–(2.9). Zero solutions of the other subproblems in (2.11)–(2.13) together with the smallest size of core problems indicate that the core problems contain all the sufficient and only the necessary information for solving the original problems (2.1)–(2.3). Further (CP1)–(CP3) imply, e.g., that:

(CP4) Matrices $[b_1, A_{11}]$, $[B_1, A_{11}]$, and $[\mathcal{B}_1^{\{1\}}, A_{11}]$ are of *full row rank* μ.

In the case of matrix right-hand side, multiplicities of singular values of A_{11} and $[B_1, A_{11}]$ are bounded by δ, etc.

It is necessary to emphasize that for the core problem with a single right-hand side, the properties (CP1)–(CP3) allow to prove that its always uniquely TLS solvable (see [18]). Let $x_{1,\mathrm{TLS}}$ be the uniquely given TLS solution of the core problem. Combining (2.7) with (2.10) (left equation) we get that the vector

$$x = Q \begin{bmatrix} x_{1,\mathrm{TLS}} \\ 0 \end{bmatrix}$$

is the TLS solution of the original problem (2.1) with minimum 2-norm (if such a solution exists), or the nongeneric solution with minimum 2-norm otherwise (see [23] for the definition of the nongeneric solution). In this way the core reduction simplifies the analysis and solution of TLS problems with $d = 1$. Note that for problems with a matrix or tensor right-hand side (see [4] and [10]) the core problem may stay unsolvable in the TLS sense.

3. Tensor models

Let us consider the matrix (multiple) right-hand side linear approximation problem $\mathcal{A}(X) \equiv AX \approx B$ (see (1.2) and (2.2)) with the linear mapping $\mathcal{A} : \mathbb{F}^{n\times d} \longrightarrow \mathbb{F}^{m\times d}$, $\mathcal{A} \in \mathscr{L}(\mathbb{F}^{n\times d}, \mathbb{F}^{m\times d})$. The vectorization of the matrices X and B rearranges

$$AX \approx B \qquad \text{to} \qquad (I \otimes A)\,\mathrm{vec}(X) \approx \mathrm{vec}(B), \tag{3.1}$$

where $\otimes$ is the Kronecker product, and $\mathrm{vec}(X)$ stacks the columns of X in one long column vector. The corrected problem $(A+E)X = B+G$ (see (1.3) and (2.5)) then becomes

$$\begin{aligned} \Big(I \otimes (A+E)\Big)\,\mathrm{vec}(X) &= \mathrm{vec}(B+G), \\ \Big(\underbrace{(I \otimes A)}_{\mathcal{A}} + \underbrace{(I \otimes E)}_{\mathcal{E}}\Big)\,\mathrm{vec}(X) &= \mathrm{vec}(B) + \mathrm{vec}(G). \end{aligned}$$

The mapping-perturbation $\mathcal{E}$ follows the Kronecker-product structure of $\mathcal{A}$.

Thus, for the matrix right-hand side TLS problem (2.5), the *search-set* $\mathscr{E}$ for the data corrections (see (1.3)) is *restricted* to an (mn)-dimensional *proper subspace* of $\mathscr{L}(\mathbb{F}^{n\times d}, \mathbb{F}^{m\times d})$ isomorphic to the vector space $\mathbb{F}^{m\times n}$ (and the subspace $\{I_d \otimes E : E \in \mathbb{F}^{m\times n}\}$ of $\mathbb{F}^{(md)\times(nd)}$). As discussed already in [5], this restriction is the key factor limiting the TLS solvability of (2.2).

One way to overcome this fundamental difficulty is to allow for more general corrections of the given data. Thus here we study several generalizations of the TLS problem (2.5) relaxing the restrictions by enriching the search-set. First, we consider a bilinear model and derive a generalization of the core reduction for this case. A note on models with *higher Kronecker rank* represented by sums of bilinear models follows. Finally, full tensor models are described; see the illustration in Fig. 1.

We show that in the case of full tensor model, the approximation problem can be interpreted (employing the vectorization similarly as in (3.1)) as the standard vector (single) right-hand side problem. There the solvability is simpler, better understood and the solution can be constructed through the unique (and always existing) solution of its core problem. Consequently, the enlargement of the search set $\mathscr{E}$ from the smallest (corresponding the standard matrix right-hand sided models (2.5)) to the largest (corresponding to the full tensor models) is accompanied by improving the TLS solvability properties of the approximation problems themselves, and also the core problems within.

3.1. Generalization to bilinear model

One of the simplest generalizations of the mapping is a modification of (3.1) to

$$A_{\mathfrak{L}} X A_{\mathfrak{R}}^* \approx B \qquad \text{or} \qquad (\overline{A_{\mathfrak{R}}} \otimes A_{\mathfrak{L}})\,\mathrm{vec}(X) \approx \mathrm{vec}(B) \tag{3.2}$$

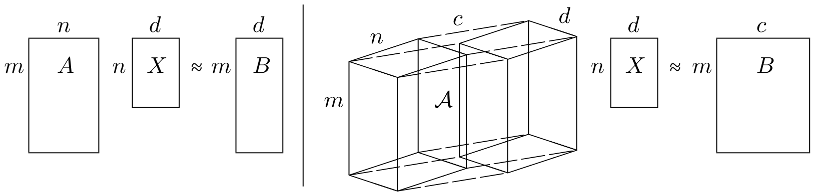

Fig. 1. Illustration of linear approximation problems with the matrix right-hand side with differently structured mapping. Left: The model is realized by the only matrix (highly structured tensor mapping). Right: The model is fully general, i.e., realized by a general tensor of fourth-order.

for a vectorization of $X \in \mathbb{F}^{n\times d}$ and $B \in \mathbb{F}^{m\times c}$. The mapping is realized by a pair of matrices $A_\mathfrak{L} \in \mathbb{F}^{m\times n}$ and $A_\mathfrak{R} \in \mathbb{F}^{c\times d}$. Such problems have been studied, e.g., in [13, Sect. 3] or [14]. A generalization of the TLS formulation is straightforward.

Definition 3.1. Let $A_\mathfrak{L} X A_\mathfrak{R}^* \approx B$ be an approximation problem (see (3.2)). The minimization problem

$$\min_{\substack{G\in\mathbb{F}^{m\times c}\\ E_\mathfrak{L}\in\mathbb{F}^{m\times n}\\ E_\mathfrak{R}\in\mathbb{F}^{c\times d}}} \left\|\begin{bmatrix} G & E_\mathfrak{L}\\ E_\mathfrak{R}^* & 0\end{bmatrix}\right\|_F \quad \text{subject to} \quad (A_\mathfrak{L}+E_\mathfrak{L})X(A_\mathfrak{R}+E_\mathfrak{R})^* = (B+G) \qquad (3.3)$$

is called the TLS problem with a bilinear model and a matrix right-hand side.

The vectorization and the corresponding rearranging then reveals the structure of the corrected problem,

$$\Big(\overline{(A_\mathfrak{R}+E_\mathfrak{R})}\otimes(A_\mathfrak{L}+E_\mathfrak{L})\Big)\operatorname{vec}(X) = \operatorname{vec}(B+G),$$

$$\Big(\underbrace{(\overline{A_\mathfrak{R}}\otimes A_\mathfrak{L})}_{\mathcal{A}}+\underbrace{(\overline{E_\mathfrak{R}}\otimes A_\mathfrak{L})+(\overline{A_\mathfrak{R}}\otimes E_\mathfrak{L})+(\overline{E_\mathfrak{R}}\otimes E_\mathfrak{L})}_{\mathcal{E}}\Big)\operatorname{vec}(X) = \operatorname{vec}(B)+\operatorname{vec}(G). \qquad (3.4)$$

One can see that the mapping-perturbation $\mathcal{E}$ now has a significantly more complicated Kronecker-product structure. With $d > 1$, the *search-set* $\mathscr{E}$ (see (1.3)) is restricted to an $(mn + cd)$-dimensional *proper submanifold* of $\mathscr{L}(\mathbb{F}^{n\times d}, \mathbb{F}^{m\times c})$ homeomorphic to the vector space $\mathbb{F}^{m\times n} \times \mathbb{F}^{c\times d} = \{(E_\mathfrak{L}, E_\mathfrak{R}) : E_\mathfrak{L} \in \mathbb{F}^{m\times n}, E_\mathfrak{R} \in \mathbb{F}^{c\times d}\}$. Note that the TLS solvability of (3.2)–(3.3) is under investigation.

Motivated by the core reduction for problems with a matrix model and matrix right-hand side [7], we want to generalize the core problem concept to (3.2). Let us consider the following unitary transformation

$$\widehat{A}_\mathfrak{L}\widehat{X}\widehat{A}_\mathfrak{R}^* \equiv (P^*A_\mathfrak{L}Q)(Q^*XR)(R^*A_\mathfrak{R}^*K) \approx (P^*BK) \equiv \widehat{B}, \qquad (3.5)$$

where $P^{-1} = P^*$, $Q^{-1} = Q^*$, $K^{-1} = K^*$, $R^{-1} = R^*$ are unitary matrices. We are looking for matrices

$$P^* B K \equiv \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad P^* A_{\mathfrak{L}} Q \equiv \begin{bmatrix} A_{\mathfrak{L},11} & 0 \\ 0 & A_{\mathfrak{L},22} \end{bmatrix}, \quad K^* A_{\mathfrak{R}} R \equiv \begin{bmatrix} A_{\mathfrak{R},11} & 0 \\ 0 & A_{\mathfrak{R},22} \end{bmatrix},$$

where B_1, $A_{\mathfrak{L},11}$, $A_{\mathfrak{R},11}$ have minimal dimensions over all unitary transformations yielding the same block structure. Conformal partitioning of $\widehat{X}$ then would split the original problem to four subproblems

$$\begin{aligned} &A_{\mathfrak{L},11} X_{11} A^*_{\mathfrak{R},11} \approx B_1 \\ \text{and} \qquad &A_{\mathfrak{L},11} X_{12} A^*_{\mathfrak{R},22} \approx 0, \quad A_{\mathfrak{L},22} X_{21} A^*_{\mathfrak{R},11} \approx 0, \quad A_{\mathfrak{L},22} X_{22} A^*_{\mathfrak{R},22} \approx 0, \end{aligned} \tag{3.6}$$

where only the first needs to be solved, since $X_{12} = 0$, $X_{21} = 0$, $X_{22} = 0$. The following definition formally introduces the desired core problem.

Definition 3.2. The subproblem

$$A_{\mathfrak{L},11} X_{11} A^*_{\mathfrak{R},11} \approx B_1$$

(see (3.6)) is called the core problem within a linear approximation problem $A_{\mathfrak{L}} X A^*_{\mathfrak{R}} \approx B$ (see (3.2)), if $A_{\mathfrak{L},11}$, $A_{\mathfrak{R},11}$ and B_1 are minimally dimensioned (and $A_{\mathfrak{L},22}$, $A_{\mathfrak{R},22}$ maximally dimensioned) subject to the unitary transformation

$$P^* B K \equiv \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad P^* A_{\mathfrak{L}} Q \equiv \begin{bmatrix} A_{\mathfrak{L},11} & 0 \\ 0 & A_{\mathfrak{L},22} \end{bmatrix}, \quad K^* A_{\mathfrak{R}} R \equiv \begin{bmatrix} A_{\mathfrak{R},11} & 0 \\ 0 & A_{\mathfrak{R},22} \end{bmatrix},$$

where $P^* = P^{-1}$, $Q^* = Q^{-1}$, $K^* = K^{-1}$, $R^* = R^{-1}$.

We show that such core problem can be revealed in three subsequent steps:

3.1.1 Transformation of the system matrices;
3.1.2 Transformation of the right-hand side; and
3.1.3 Final permutation.

Note that in the standard matrix (multiple) right-hand side case an extra step of right-hand side preprocessing is required; see [7]. This part can be skipped here since the transformation of B is realized implicitly during the other steps. We now describe the process in detail.

3.1.1. Transformation of the system matrices

We start with modification of the model matrices to simplest, in particular diagonal, forms. Consider the SVDs of $A_{\mathfrak{L}}$ and $A_{\mathfrak{R}}$,

$$\begin{aligned} A_{\mathfrak{L}} &= U_{\mathfrak{L}}\Sigma V_{\mathfrak{L}}^*, & U_{\mathfrak{L}} &\in \mathbb{F}^{m\times m}, & \Sigma &\in \mathbb{R}^{m\times n}, & V_{\mathfrak{L}} &\in \mathbb{F}^{n\times n},\\ A_{\mathfrak{R}} &= U_{\mathfrak{R}}\Psi V_{\mathfrak{R}}^*, & U_{\mathfrak{R}} &\in \mathbb{F}^{c\times c}, & \Psi &\in \mathbb{R}^{c\times d}, & V_{\mathfrak{R}} &\in \mathbb{F}^{d\times d}, \end{aligned} \tag{3.7}$$

where $U_{\mathfrak{L}}^* = U_{\mathfrak{L}}^{-1}$, $V_{\mathfrak{L}}^* = V_{\mathfrak{L}}^{-1}$, $U_{\mathfrak{R}}^* = U_{\mathfrak{R}}^{-1}$, $V_{\mathfrak{R}}^* = V_{\mathfrak{R}}^{-1}$. Let $A_{\mathfrak{L}}$ and $A_{\mathfrak{R}}$ have ξ and ζ *distinct* nonzero singular values

$$\sigma_1 > \sigma_2 > \cdots > \sigma_\xi > 0 \qquad \text{and} \qquad \psi_1 > \psi_2 > \cdots > \psi_\zeta > 0, \tag{3.8}$$

and let m_i, $i = 1, \ldots, \xi$, and c_j, $j = 1, \ldots, \zeta$ be their multiplicities, respectively, i.e., $\sum_{i=1}^{\xi} m_i = \operatorname{rank}(A_{\mathfrak{L}})$ and $\sum_{j=1}^{\zeta} c_j = \operatorname{rank}(A_{\mathfrak{R}})$. Further denote $m_{\xi+1} \equiv m - \operatorname{rank}(A_{\mathfrak{L}})$, $n_{\xi+1} \equiv n - \operatorname{rank}(A_{\mathfrak{L}})$, $c_{\zeta+1} \equiv c - \operatorname{rank}(A_{\mathfrak{R}})$, and $d_{\zeta+1} \equiv d - \operatorname{rank}(A_{\mathfrak{R}})$. The problem (3.2) can be then transformed to

$$(U_{\mathfrak{L}}^* A_{\mathfrak{L}} V_{\mathfrak{L}}) Z (V_{\mathfrak{R}}^* A_{\mathfrak{R}}^* U_{\mathfrak{R}}) = \Sigma Z \Psi^{\mathsf{T}} \approx F, \quad \text{where} \quad F \equiv U_{\mathfrak{L}}^* B U_{\mathfrak{R}}, \quad Z \equiv V_{\mathfrak{L}}^* X V_{\mathfrak{R}}. \tag{3.9}$$

Both system matrices are now *diagonal*.

3.1.2. Transformation of the right-hand side

Next, we need to get as many zero rows and columns in the right-hand side as possible, while preserving the diagonal structure of the system matrices. Consider the partitioning

$$F = \begin{bmatrix} F_{1,1} & \cdots & F_{1,\zeta+1} \\ \vdots & \ddots & \vdots \\ F_{\xi+1,1} & \cdots & F_{\xi+1,\zeta+1} \end{bmatrix}, \quad \text{where} \quad F_{i,j} \in \mathbb{F}^{m_i \times c_j}, \tag{3.10}$$

$i = 1, 2, \ldots, \xi, \xi+1$, $j = 1, 2, \ldots, \zeta, \zeta+1$. Denote μ_i and γ_j ranks of individual block-rows and block-columns of F, respectively. Consider the following two sets of SVDs

$$\begin{aligned} \left[F_{i,1}, \ldots, F_{i,\zeta+1} \right] &= S_{\mathfrak{L},i} \Theta_{\mathfrak{L},i} W_{\mathfrak{L},i}^*, \quad S_{\mathfrak{L},i} \in \mathbb{F}^{m_i \times m_i}, \quad \Theta_{\mathfrak{L},i} \in \mathbb{R}^{m_i \times \mu_i}, \quad W_{\mathfrak{L},i} \in \mathbb{F}^{c \times \mu_i}, \\ \begin{bmatrix} F_{1,j} \\ \vdots \\ F_{\xi+1,j} \end{bmatrix} &= S_{\mathfrak{R},j} \Theta_{\mathfrak{R},j} W_{\mathfrak{R},j}^*, \quad S_{\mathfrak{R},j} \in \mathbb{F}^{m \times \gamma_j}, \quad \Theta_{\mathfrak{R},j} \in \mathbb{R}^{\gamma_j \times c_j}, \quad W_{\mathfrak{R},j} \in \mathbb{F}^{c_j \times c_j}, \end{aligned}$$

where $S_{\mathfrak{L},i}^* = S_{\mathfrak{L},i}^{-1}$, $W_{\mathfrak{R},j}^* = W_{\mathfrak{R},j}^{-1}$ are square unitary matrices, $\Theta_{\mathfrak{L},i}$ is of full column rank μ_i, $\Theta_{\mathfrak{R},j}$ is of full row rank γ_j, and $W_{\mathfrak{L},i}$, $S_{\mathfrak{R},j}$ have mutually orthonormal columns, i.e., $W_{\mathfrak{L},i}^* W_{\mathfrak{L},i} = I_{\mu_i}$, $S_{\mathfrak{R},j}^* S_{\mathfrak{R},j} = I_{\gamma_j}$. Define unitary matrices

$$\begin{aligned} S_U &\equiv \operatorname{diag}(S_{\mathfrak{L},1}, \ldots, S_{\mathfrak{L},\xi}, S_{\mathfrak{L},\xi+1}), & S_V &\equiv \operatorname{diag}(S_{\mathfrak{L},1}, \ldots, S_{\mathfrak{L},\xi}, I_{n_{\xi+1}}), \\ W_U &\equiv \operatorname{diag}(W_{\mathfrak{R},1}, \ldots, W_{\mathfrak{R},\zeta}, W_{\mathfrak{R},\zeta+1}), & W_V &\equiv \operatorname{diag}(W_{\mathfrak{R},1}, \ldots, W_{\mathfrak{R},\zeta}, I_{d_{\zeta+1}}). \end{aligned} \tag{3.11}$$

Since $S_U^* \Sigma S_V = \Sigma$ and $W_U^* \Psi W_V = \Psi$, the problem (3.9) can be transformed to

$$(S_U^* \Sigma S_V)(S_V^* Z W_V)(W_V^* \Psi^{\mathsf{T}} W_U) = \Sigma (S_V^* Z W_V) \Psi^{\mathsf{T}} \approx (S_U^* F W_U), \tag{3.12}$$

while preserving the structure of system matrices, and producing the right-hand side

$$S_U^* F W_U = \begin{bmatrix} S_{\mathfrak{L},1}^* F_{1,1} W_{\mathfrak{R},1} & \cdots & S_{\mathfrak{L},1}^* F_{1,\zeta+1} W_{\mathfrak{R},\zeta+1} \\ \vdots & \ddots & \vdots \\ S_{\mathfrak{L},\xi+1}^* F_{\xi+1,1} W_{\mathfrak{R},1} & \cdots & S_{\mathfrak{L},\xi+1}^* F_{\xi+1,\zeta+1} W_{\mathfrak{R},\zeta+1} \end{bmatrix}.$$

The matrices

$$S_{\mathfrak{L},i}^* \Big[F_{i,1}, \ldots, F_{i,\zeta+1} \Big] = \Theta_{\mathfrak{L},i} W_{\mathfrak{L},i}^* \qquad \text{and} \qquad \begin{bmatrix} F_{1,j} \\ \vdots \\ F_{\xi+1,j} \end{bmatrix} W_{\mathfrak{R},j} = S_{\mathfrak{R},j} \Theta_{\mathfrak{R},j}$$

have μ_i nonzero and mutually orthogonal rows (followed by $m_i - \mu_i$ zero rows), and γ_j nonzero and mutually orthogonal columns (followed by $c_j - \gamma_j$ zero columns), respectively. Thus

$$S_{\mathfrak{L},i}^* F_{i,j} W_{\mathfrak{R},j} \equiv \begin{bmatrix} H_{i,j} & 0_{m_i, c_j - \gamma_j} \\ 0_{m_i - \mu_i, \gamma_j} & 0_{m_i - \mu_i, c_j - \gamma_j} \end{bmatrix}, \qquad H_{i,j} \in \mathbb{F}^{\mu_i \times \gamma_j}, \tag{3.13}$$

and also $[H_{i,1}, \ldots, H_{i,\zeta+1}]$ and $[H_{1,j}^{\mathsf{T}}, \ldots, H_{\xi+1,j}^{\mathsf{T}}]^{\mathsf{T}}$ are of *full row rank, having mutually orthogonal rows.*

3.1.3. Final permutation

Finally, we construct permutation matrices in order to aggregate the relevant information revealed in the nonzero blocks of the right-hand side, while still keeping the system matrices as diagonal as possible. Let us consider two pairs of permutation matrices

$$\Pi_{\mathfrak{L},U} \equiv \left[\begin{array}{cccc|cccc} \begin{bmatrix} I_{\mu_1} \\ 0 \end{bmatrix} & & 0 & 0 & \begin{bmatrix} 0 \\ I_{m_1-\mu_1} \end{bmatrix} & & 0 & 0 \\ & \ddots & & \vdots & & \ddots & & \vdots \\ 0 & & \begin{bmatrix} I_{\mu_\xi} \\ 0 \end{bmatrix} & 0 & 0 & & \begin{bmatrix} 0 \\ I_{m_\xi-\mu_\xi} \end{bmatrix} & 0 \\ 0 & \cdots & 0 & \begin{bmatrix} I_{\mu_{\xi+1}} \\ 0 \end{bmatrix} & 0 & \cdots & 0 & \begin{bmatrix} 0 \\ I_{m_{\xi+1}-\mu_{\xi+1}} \end{bmatrix} \end{array} \right],$$

$$\Pi_{\mathfrak{L},V} \equiv \left[\begin{array}{ccc|cccc} \begin{bmatrix} I_{\mu_1} \\ 0 \end{bmatrix} & & 0 & \begin{bmatrix} 0 \\ I_{m_1-\mu_1} \end{bmatrix} & & 0 & 0 \\ & \ddots & & & \ddots & & \vdots \\ 0 & & \begin{bmatrix} I_{\mu_\xi} \\ 0 \end{bmatrix} & 0 & & \begin{bmatrix} 0 \\ I_{m_\xi-\mu_\xi} \end{bmatrix} & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & I_{n_{\xi+1}} \end{array} \right],$$

and $\Pi_{\mathfrak{R},U}$, $\Pi_{\mathfrak{R},V}$; the second pair is fully analogous to the first, but with ms, ns, μs, and ξs replaced by cs, ds, γs, and ζs, respectively.

Recall that the steps (3.9) and (3.12) together transform the original problem (3.2) to

$$\underbrace{(S_U^* U_{\mathfrak{L}}^* A_{\mathfrak{L}} V_{\mathfrak{L}} S_V)}_{\Sigma}(S_V^* V_{\mathfrak{L}}^* X V_{\mathfrak{R}} W_V)\underbrace{(W_V^* V_{\mathfrak{R}}^* A_{\mathfrak{R}}^* U_{\mathfrak{R}} W_U)}_{\Psi^{\mathsf{T}}} \approx (S_U^* U_{\mathfrak{L}}^* B U_{\mathfrak{R}} W_U). \tag{3.14}$$

Then

$$\Pi_{\mathfrak{L},U}^{\mathsf{T}}(S_U^* U_{\mathfrak{L}}^* A_{\mathfrak{L}} V_{\mathfrak{L}} S_V)\Pi_{\mathfrak{L},V} = \operatorname{diag}\Big(\overbrace{\operatorname{diag}(\sigma_1 I_{\mu_1}, \sigma_2 I_{\mu_2}, \ldots, \sigma_\xi I_{\mu_\xi}, 0_{\mu_{\xi+1},0})}^{A_{\mathfrak{L},11}},$$

$$\underbrace{\operatorname{diag}(\sigma_1 I_{m_1-\mu_1}, \sigma_2 I_{m_2-\mu_2}, \ldots, \sigma_\xi I_{m_\xi-\mu_\xi}, 0_{m_{\xi+1}-\mu_{\xi+1},n_{\xi+1}})}_{A_{\mathfrak{L},22}} \Big) \equiv \begin{bmatrix} A_{\mathfrak{L},11} & 0 \\ 0 & A_{\mathfrak{L},22} \end{bmatrix},$$

$$\Pi_{\mathfrak{R},U}^{\mathsf{T}}(W_U^* U_{\mathfrak{R}}^* A_{\mathfrak{R}} V_{\mathfrak{R}} W_V)\Pi_{\mathfrak{R},V} = \operatorname{diag}\Big(\overbrace{\operatorname{diag}(\psi_1 I_{\gamma_1}, \psi_2 I_{\gamma_2}, \ldots, \psi_\zeta I_{\gamma_\zeta}, 0_{0,\gamma_{\zeta+1}})}^{A_{\mathfrak{R},11}},$$

$$\underbrace{\operatorname{diag}(\psi_1 I_{c_1-\gamma_1}, \psi_2 I_{c_2-\gamma_2}, \ldots, \psi_\zeta I_{c_\zeta-\gamma_\zeta}, 0_{d_{\zeta+1},c_{\zeta+1}-\gamma_{\zeta+1}})}_{A_{\mathfrak{R},22}} \Big) \equiv \begin{bmatrix} A_{\mathfrak{R},11} & 0 \\ 0 & A_{\mathfrak{R},22} \end{bmatrix},$$

and

$$\Pi_{\mathfrak{L},U}^{\mathsf{T}}(S_U^* U_{\mathfrak{L}}^* B U_{\mathfrak{R}} W_U)\Pi_{\mathfrak{R},U} = \begin{bmatrix} H_{1,1} & \cdots & H_{1,\zeta+1} & 0 \\ \vdots & \ddots & \vdots & \vdots \\ H_{\xi+1,1} & \cdots & H_{\xi+1,\zeta+1} & 0 \\ 0 & \cdots & 0 & 0 \end{bmatrix} \equiv \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{3.15}$$

3.1.4. Summary of the transformation

The whole core problem reduction can be summarized in the following key steps:

$$\begin{aligned}
A_{\mathfrak{L}} X A_{\mathfrak{R}}^* &\approx B && \text{(see (3.2))},\\
\underbrace{(U_{\mathfrak{L}}^* A_{\mathfrak{L}} V_{\mathfrak{L}})}_{\Sigma}\underbrace{(V_{\mathfrak{L}}^* X V_{\mathfrak{R}})}_{Z}\underbrace{(U_{\mathfrak{R}}^* A_{\mathfrak{R}} V_{\mathfrak{R}})}_{\Psi}{}^* &\approx \underbrace{U_{\mathfrak{L}}^* B U_{\mathfrak{R}}}_{F} && \text{(see (3.9))},\\
\overbrace{(S_U^* \Sigma S_V)}(S_V^* Z W_V)\overbrace{(W_U^* \Psi W_V)}{}^* &\approx S_U^* F W_U && \text{(see (3.12), (3.14))},\\
\underbrace{(\Pi_{\mathfrak{L},U}^{\mathsf{T}} \Sigma \Pi_{\mathfrak{L},V})}_{\begin{bmatrix} A_{\mathfrak{L},11} & 0 \\ 0 & A_{\mathfrak{L},22} \end{bmatrix}}\underbrace{(\Pi_{\mathfrak{L},V}^{\mathsf{T}} S_V^* Z W_V \Pi_{\mathfrak{R},V})}_{\begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}}\underbrace{(\Pi_{\mathfrak{R},U}^{\mathsf{T}} \Psi \Pi_{\mathfrak{R},V})}_{\begin{bmatrix} A_{\mathfrak{R},11}^* & 0 \\ 0 & A_{\mathfrak{R},22}^* \end{bmatrix}}{}^* &\approx \underbrace{\Pi_{\mathfrak{L},U}^{\mathsf{T}} S_U^* F W_U \Pi_{\mathfrak{R},U}}_{\begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}}, \;\; .
\end{aligned}$$

A comparison with (3.5) gives the transformation matrices

$$P \equiv U_{\mathfrak{L}} S_U \Pi_{\mathfrak{L},U}, \quad Q \equiv V_{\mathfrak{L}} S_V \Pi_{\mathfrak{L},V}, \quad K \equiv U_{\mathfrak{R}} W_U \Pi_{\mathfrak{R},U}, \quad \text{and} \quad R \equiv V_{\mathfrak{R}} W_V \Pi_{\mathfrak{R},V}.$$

Moreover, the constructed problem has several notable properties:

(CP1) Matrices $A_{\mathfrak{L},11}$ and $A_{\mathfrak{R},11}$ are of *full column rank.*

(CP2–3)[2] Let $A_{\mathfrak{L},11}$ have ξ distinct singular values with multiplicities μ_i and $\mu_{\xi+1} \equiv \dim(\mathscr{N}(A^*_{\mathfrak{L},11}))$, and let $U_{\mathfrak{L},i}$ be matrices having orthonormal bases of left singular vector subspaces of $A_{\mathfrak{L},11}$ as their columns.

Let $A_{\mathfrak{R},11}$ have ζ distinct singular values with multiplicities γ_j and $\gamma_{\zeta+1} \equiv \dim(\mathscr{N}(A^*_{\mathfrak{R},11}))$, and let $U_{\mathfrak{R},j}$ be matrices having orthonormal bases of left singular vector subspaces of $A_{\mathfrak{R},11}$ as their columns.

The matrices $U^*_{\mathfrak{L},i}B_1$ are of *full row rank* μ_i, $i = 1, 2, \ldots, \xi, \xi + 1$, and $B_1 U_{\mathfrak{R},j}$ of *full column rank* γ_j, $j = 1, 2, \ldots, \zeta, \zeta + 1$; see (3.15).

These properties further imply in particular:

(CP4) Matrices $[B_1, A_{\mathfrak{L},11}]$ and $[B_1^*, A_{\mathfrak{R},11}]$ are of *full row rank.*

Note that in the standard matrix right-hand side case, the preprocessing ensures that B_1 is of full column rank (possibly having mutually orthogonal columns). Here we obtained B_1 with block-columns having this property; the size of these block-columns is given by the multiplicities of singular values of $A_{\mathfrak{R}}$. Clearly, by considering $c = d$ and $A_{\mathfrak{R}} \equiv I_d$ we get the standard preprocessed core problem within $A_{\mathfrak{L}} X A^*_{\mathfrak{R}} = A_{\mathfrak{L}} X I_d = A_{\mathfrak{L}} X \approx B$ as in [7].

In [7, Sect. 4.1, pp. 926–929], it was shown that for the matrix right-hand side case the properties (CP1)–(CP3) imply the minimality of the obtained subproblem and thus ensure that the transformation is the core reduction. The following theorem summarizes analogous result for the transformation derived above. The proof is a generalization of the proof from [7], thus we omit it here.

Theorem 3.3. *The unitary transformation developed in sections 3.1.1–3.1.3 is the core problem revealing transformation, i.e., the system matrices $A_{\mathfrak{L},11}$, $A_{\mathfrak{R},11}$ and the right-hand side matrix B_1 form the core problem*

$$A_{\mathfrak{L},11} X_{11} A^*_{\mathfrak{R},11} \approx B_1$$

within $A_{\mathfrak{L}} X A^*_{\mathfrak{R}} \approx B$.

Consequently, for the approximation problems with multiple observations on bilinear models, we are able to extract necessary and sufficient information analogously as in [7] for matrix models. It is worth to note that similarly as in the matrix case, the existence of a TLS solution of the core problem given in Theorem 3.3 is not ensured; see [4] or [11] for the detailed analysis of solvability of matrix core problems.

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[2] The properties (CP2) and (CP3) (see section 2.2, or [7, p. 925], or [4, p. 864]) here coincide while being denoted (CP2–3) both together.

3.2. Note on models with higher Kronecker rank

The next step in generalization of problems (3.1) and (3.2) (while further enlarging the search-set) can be considering a sum of several bilinear models

$$\sum_{\ell=1}^{L} A_{\mathfrak{L},\ell} X A_{\mathfrak{R},\ell}^{*} \approx B, \qquad \text{or} \qquad \Big(\sum_{\ell=1}^{L} (\overline{A_{\mathfrak{R},\ell}} \otimes A_{\mathfrak{L},\ell}) \Big) \operatorname{vec}(X) \approx \operatorname{vec}(B), \tag{3.16}$$

after a vectorization of $X \in \mathbb{F}^{n \times d}$ and $B \in \mathbb{F}^{m \times c}$. The mapping is realized by L pairs of matrices $A_{\mathfrak{L},\ell} \in \mathbb{F}^{m \times n}$ and $A_{\mathfrak{R},\ell} \in \mathbb{F}^{c \times d}$, simply saying it is of Kronecker rank L.

Problems (3.2) and (3.16) differ only in the number of summands on the left-hand side. Thus, a TLS problem can be defined analogously to the Definition 3.1. On the other hand, the generalization of the core problem reduction is questionable, since for $L \geq 2$ the left (and also right) matrices $A_{\mathfrak{L},\ell}$ ($A_{\mathfrak{R},\ell}$) have in general no common singular vectors, i.e., no common SVD. For $L = 2$ one could consider the so-called generalized SVD (GSVD) (see, e.g., [3, Sect. 6.1.6, pp. 309–311]) which delivers a common SVD-like decomposition of a pair of matrices, e.g., in the form $A_{\mathfrak{L},1} = U_1 \Sigma_1 V^{-1}$ and $A_{\mathfrak{L},2} = U_2 \Sigma_2 V^{-1}$. However, the common factor V is not unitary and thus it does not preserve the (Frobenius) norm used in the minimization in the TLS formulation.

We see that the generalization of the core reduction would require for example some symmetry to be present in (3.16). This is the case when the problem contains only two summands on the left-hand side ($L = 2$) with two pairs of matrices conjugated to each other (possibly up to a sign) or, moreover, with two of them being identities. This includes in particular the cases

$$\begin{array}{lll} AX + XM^* \approx B, & AX \pm XA^* \approx B, & AXM^* \pm MXA^* \approx B, \\ AXM^* + X \approx B, & AXA^* \pm X \approx B, & AXA^* \pm MXM^* \approx B, \end{array} \tag{3.17}$$

i.e., the problems resemble the Sylvester, Lyapunov, or generalized Lyapunov equation in its continuous or discrete form.

3.3. Generalization to full tensor model

Now we turn to a fully general linear mapping $\mathcal{A} \in \mathscr{L}(\mathbb{F}^{n \times d}, \mathbb{F}^{m \times c})$ represented by a tensor of fourth order. Consider a general linear approximation problem (1.2) of the form

$$\mathcal{A} \times_{((3,4),(1,2))} X \approx B, \qquad \text{where} \qquad \mathcal{A} \in \mathbb{F}^{m \times c \times n \times d}, \quad X \in \mathbb{F}^{n \times d}, \quad B \in \mathbb{F}^{m \times c}, \tag{3.18}$$

and the product $\times_{((3,4),(1,2))}$ means that the third- and fourth-mode fibres of the object on its left are multiplied with the first- and second-mode fibres of the object on its right, respectively. Then (3.18) can be rewritten in the componentwise notation as

$$\sum_{k=1}^{n}\sum_{l=1}^{d} a_{i,j,k,l}\cdot x_{k,l} \approx b_{i,j}, \qquad \text{or} \qquad \sum_{(k,l)=(1,1)}^{(n,d)} a_{(i,j),(k,l)}\cdot x_{(k,l)} \approx b_{(i,j)}$$

or employing multiindices (i,j) and (k,l) sorted in the lexicographical order. The last notation is in fact the standard matrix-vector product of a matrix $\mathcal{A}^{\{1,2\}} \in \mathbb{F}^{(mc)\times(nd)}$ having entries $a_{(i,j),(k,l)}$ on the (i,j)th row and (k,l)th column, the so-called $\{1,2\}$-*modes matricization* of the tensor $\mathcal{A}$, and the long vector $\operatorname{vec}(X) \in \mathbb{F}^{(nd)}$ having entries $x_{(k,l)}$. Consequently, we formally get

$$\mathcal{A}^{\{1,2\}}\operatorname{vec}(X) \approx \operatorname{vec}(B). \tag{3.19}$$

All previously discussed approximation problems are special cases of (3.19). A comparison of (3.19) with (3.1), (3.2), and (3.16) reveals that in those cases, the fourth-order tensor $\mathcal{A}$ has a specific structure, namely

$$\mathcal{A}^{\{1,2\}} = I\otimes A, \quad \text{or} \quad \overline{A_{\mathfrak{R}}}\otimes A_{\mathfrak{L}}, \quad \text{or} \quad \sum_{\ell=1}^{L}\overline{A_{\mathfrak{R},\ell}}\otimes A_{\mathfrak{L},\ell} \in \mathbb{F}^{(mc)\times(nd)}.$$

Furthermore, in the important cases of Sylvester-like or Lyapunov-like problems (3.17), we have

$$\begin{aligned}\mathcal{A}^{\{1,2\}} = (I\otimes A) + (\overline{M}\otimes I), &\quad (I\otimes A) \pm (\overline{A}\otimes I), \quad (\overline{M}\otimes A) \pm (\overline{A}\otimes M),\\ (\overline{M}\otimes A) + (I\otimes I), &\quad (\overline{A}\otimes A) \pm (I\otimes I), \quad (\overline{A}\otimes A) \pm (\overline{M}\otimes M).\end{aligned}$$

Obviously, the tensors $\mathcal{A}$ above are highly structured and symmetric. This structure can also be seen by using the $\{1,3\}$-modes matricization of $\mathcal{A}$, i.e., $a_{i,j,k,l}$ is in the matrix $\mathcal{A}^{\{1,3\}} \in \mathbb{F}^{(mn)\times(cd)}$ placed in the (i,k)th row and (j,l)th column. Then

$$\mathcal{A}^{\{1,3\}} = \operatorname{vec}(A)\operatorname{vec}(I)^{\mathsf{T}}, \quad \operatorname{vec}(A_{\mathfrak{L}})\operatorname{vec}(A_{\mathfrak{R}})^{*}, \quad \sum_{\ell=1}^{L}\operatorname{vec}(A_{\mathfrak{L},\ell})\operatorname{vec}(A_{\mathfrak{R},\ell})^{*},$$

which is a rank-one matrix for problems (3.1) and (3.2), and at most rank L matrix for problem (3.16). Similarly, for the Sylvester-like and Lyapunov-like problems (3.17) the matrix is of rank at most two.

Concerning the TLS definition for (3.2) introduced in Definition 3.1 (and its analogy for (3.16)), it is important to note that whenever X is multiplied from both sides, the componentwise corrections of the individual matrices $A_{\mathfrak{L}}$, $A_{\mathfrak{R}}$, $A_{\mathfrak{L},\ell}$, $A_{\mathfrak{R},\ell}$ do not represent direct componentwise corrections of the tensor; see in particular (3.4). For example, based on the $\{1,3\}$-modes matricization one can see, that the correction in the case (3.2)–(3.4) represents a *rank-three update* of the tensor $\mathcal{A}$. We now follow a different idea, where such restrictions on corrections allowed for the model are not present.

3.3.1. TLS definition and basic solvability results

The following definition introduces a TLS formulation for the general problem (3.18).

Definition 3.4. Let $\mathcal{A} \times_{((3,4),(1,2))} X \approx B$ be an approximation problem (see (3.18)). The minimization problem

$$\min_{\substack{G \in \mathbb{F}^{m \times c} \\ \mathcal{E} \in \mathbb{F}^{m \times c \times n \times d}}} \quad (\|G\|_F^2 + \|\mathcal{E}\|^2)^{\frac{1}{2}} \quad \text{subject to} \quad (\mathcal{A} + \mathcal{E}) \times_{((3,4),(1,2))} X = B + G \tag{3.20}$$

is called the full-tensor-mapping TLS problem with a matrix right-hand side.

In the definition above, the search-set $\mathscr{E}$ of the mapping-perturbation $\mathcal{E}$ (see (1.3)) covers the whole space $\mathscr{L}(\mathbb{F}^{n \times d}, \mathbb{F}^{m \times c})$, contrary to the cases discussed in the previous sections. This fact is particularly important, because the richness of the set $\mathscr{E}$ allows us to reshape (3.18) based on (3.19) into a vector (single) right-hand side problem representing the simplest and well studied case of TLS problems.

Theorem 3.5. *Let (3.18)–(3.20) be a matrix right-hand side TLS problem with a general tensor mapping. Let (2.1)–(2.4) be the corresponding vector right-hand side TLS problem with*

$$\begin{aligned} A \equiv \mathcal{A}^{\{1,2\}}, \quad E \equiv \mathcal{E}^{\{1,2\}} \in \mathbb{F}^{(mc) \times (nd)}, \quad & x \equiv \operatorname{vec}(X) \in \mathbb{F}^{nd}, \\ \text{and} \qquad b \equiv \operatorname{vec}(B), \quad & g \equiv \operatorname{vec}(G) \in \mathbb{F}^{mc}, \end{aligned} \tag{3.21}$$

i.e., A is the $\{1,2\}$-matricization of $\mathcal{A}$, and x, b, and g are vectorizations of matrices X, B, and G, respectively. Then these two TLS problems are equivalent, i.e., x represents a TLS solution of (2.1)–(2.4) if and only if X represents a TLS solution of (3.18)–(3.20).

Proof. Since matricization and vectorization represent only a reshaping of arrays, we only focus on the minimization. The search-set for mapping perturbations covers the whole space of all linear mappings in both cases. Since the norm is in both cases essentially the same, we directly get

$$\|[g, E]\|_F = (\|g\|_2^2 + \|E\|_F^2)^{\frac{1}{2}} = (\|\operatorname{vec}(G)\|_2^2 + \|\mathcal{E}^{\{1,2\}}\|_F^2)^{\frac{1}{2}} = (\|G\|_F^2 + \|\mathcal{E}\|^2)^{\frac{1}{2}}$$

which finishes the proof. □

Note that an analogous result can be formulated in a slightly more general way. If the search-set $\mathscr{E}$ for the mapping-perturbation $\mathcal{E}$ in (1.3) covers the whole space of all linear mappings $\mathscr{L}(\mathscr{U}, \mathscr{V})$, then the TLS problem can be reformulated as a vector (single) right-hand side problem (2.1)–(2.4).

Consequently, basic solvability results available for vector right-hand side TLS problems (see, e.g., [2], [23]) can be transferred to TLS problems defined in Definition 3.4 for full tensor models and a matrix right-hand side. For the vectorized problem (3.19), there is also a core reduction available with the resulting core problem having the unique TLS solution; see [18]. Note that there are questions related to the meaning of the vectorized core reduction if the original problem has some structured form, as indicated by the analysis in [10] for problems with structured right-hand sides.

3.3.2. Relation of generalization approaches

In the view of Theorem 3.5, it is interesting to observe that the problem (3.18) with the full tensor mapping can be always rewritten to the form (3.16) with a sum of bilinear models.

Let us consider the $(1,3)$-modes slices of $\mathcal{A} \in \mathbb{F}^{m\times c\times n\times d}$, i.e., (cd) subarrays in $\mathbb{F}^{m\times 1\times n\times 1}$. Denote $A_{:,j,:,l} \in \mathbb{F}^{m\times n}$ a matrix trivially isomorphic with the (j,l)th $(1,3)$-modes slice, $j = 1,2,\ldots,c$, $l = 1,2,\ldots,d$. Then the matricization $\mathcal{A}^{\{1,2\}}$ represents a two-way array of these matrices

$$\mathcal{A}^{\{1,2\}} = \begin{bmatrix} A_{:,1,:,1} & \cdots & A_{:,1,:,d} \\ \vdots & \ddots & \vdots \\ A_{:,c,:,1} & \cdots & A_{:,c,:,d} \end{bmatrix} = \sum_{j=1}^{c}\sum_{l=1}^{d}\Big(M_{j,l}\otimes A_{:,j,:,l}\Big), \qquad M_{j,l} \equiv e_j^{(c)} e_l^{(d)\mathsf{T}} \in \mathbb{R}^{c\times d},$$

where $e_k^{(\ell)}$ stands for the ith Euclidean vector of length ℓ, i.e., the ith column of I_ℓ. Thus the problem $\mathcal{A}\times_{((3,4),(1,2))} X \approx B$ can be, after a vectorization

$$\mathcal{A}^{\{1,2\}}\,\mathrm{vec}(X) \approx \mathrm{vec}(B), \quad \text{reshaped back to} \quad \sum_{j=1}^{c}\sum_{l=1}^{d} A_{:,j,:,l} X M_{j,l}^{\mathsf{T}} \approx B. \tag{3.22}$$

We see that (3.22) has now the same structure as (3.16) with $L = cd$, $A_{\mathfrak{L},\ell}$ being $(1,3)$-modes slices of $\mathcal{A}$, and $A_{\mathfrak{R},\ell}$ forming the Euclidean basis of $\mathbb{F}^{c\times d}$. This links the full tensor problem (3.18) back to the structured problem (3.16).

However, there is a substantial difference between the approach represented by a subsequent generalization of the TLS formulations from (3.1), through (3.2), to (3.16), and the TLS formulation represented by Definition 3.4. Following (3.22), the corrected system (3.20) is reshaped from

$$(\mathcal{A}+\mathcal{E})\times_{((3,4),(1,2))} X \approx (B+G) \quad \text{to} \quad \sum_{j=1}^{c}\sum_{l=1}^{d}(A_{:,j,:,l}+E_{:,j,:,l})XM_{j,l}^{\mathsf{T}} \approx (B+G).$$

Thus here the mapping-perturbation $\mathcal{E}$ *affects only the matrices on the left of* X, on the *contrary* to formulations analyzed in sections 3.1 and 3.2. We see that this last TLS formulation does not follow the nested structure of the previous generalizations. On the other hand, the search-set $\mathscr{E}$ now covers the whole space $\mathscr{L}(\mathbb{F}^{n\times d},\mathbb{F}^{m\times c})$.

4. Conclusions

We have shown that the standard matrix right-hand side TLS problem $AX \approx B$, where the model is realized by a single matrix A (i.e., by the "one-side-product"), can be extended in several ways. First, we considered the bilinear model represented by a pair of matrices, defined a straightforward TLS minimization problem and derived the core reduction for this case. Generalization to problems with a sum of bilinear models was discussed. Then, a fully general tensorized model was introduced allowing to reshape (vectorize) the problem to a single right-hand side approximation problem. Thus, some of the TLS solvability results available for $d = 1$ can be adopted to this generalization. The whole analysis shows how the properties of the model (mapping) influence the TLS minimization for the corresponding approximation problem. In particular, it was proved that the presented enlargements of the search set $\mathscr{E}$ for the model corrections result in changes in the TLS solvability of the approximation problems (and the same holds for their core problems). This work, together with the results obtained in [10], represents another step towards investigation of a fully tensorized (general as well as structured) linear approximation problem

$$\mathcal{A} \times_{((s-t+1,\ldots,s),(1,\ldots,t))} \mathcal{X} \approx \mathcal{B},$$

where the model $\mathcal{A}$ and the unknowns $\mathcal{X}$ are s-way and k-way tensors, respectively, multiplied in t modes, $t \leq \min\{s, k\}$, and the right-hand side $\mathcal{B}$ is a $(s + k - 2t)$-way tensor.

Conflict of interest statement

The authors confirm that there are no known conflicts of interest associated with this publication.

Acknowledgements

The authors wish to thank the anonymous referee for her/his helpful comments which have led to improvements of this manuscript.

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SIAM J. MATRIX ANAL. APPL.
Vol. 44, No. 1, pp. 53-79

KRYLOV SUBSPACE APPROACH TO CORE PROBLEMS WITHIN MULTILINEAR APPROXIMATION PROBLEMS: A UNIFYING FRAMEWORK*

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Abstract. Error contaminated linear approximation problems appear in a large variety of applications. The presence of redundant or irrelevant data complicates their solution. It was shown that such data can be removed by the core reduction yielding a minimally dimensioned subproblem called the core problem. Direct (SVD or Tucker decomposition-based) reduction has been introduced previously for problems with matrix models and vector, or matrix, or tensor observations; and also for problems with bilinear models. For the cases of vector and matrix observations a Krylov subspace method, the generalized Golub–Kahan bidiagonalization, can be used to extract the core problem. In this paper, we first unify previously studied variants of linear approximation problems under the general framework of a multilinear approximation problem. We show how the direct core reduction can be extended to it. Then we show that the generalized Golub–Kahan bidiagonalization yields the core problem for any multilinear approximation problem. This further allows one to prove various properties of core problems, in particular, we give upper bounds on the multiplicity of singular values of reduced matrices.

Key words. (multi)linear approximation problems, error-in-variables modeling, total least squares, core problem, orthogonal transformations, Krylov subspace methods

MSC codes. 15A06, 15A18, 15A21, 15A24, 65F20, 65F25

DOI. 10.1137/21M1462155

1. Introduction.

During the last decades, wide attention has been given to the analysis and solution of linear approximation problems contaminated by errors in the data. Generally, they can be formulated as

$$\mathcal{A}(\mathfrak{X}) \approx \mathfrak{B}, \quad \mathcal{A} \in \mathscr{L}(\mathscr{U}, \mathscr{V}), \quad \mathfrak{X} \in \mathscr{U}, \quad \mathfrak{B} \in \mathscr{V}, \tag{1.1}$$

where $\mathcal{A} : \mathscr{U} \longrightarrow \mathscr{V}$ is a given linear mapping (model) between two finite-dimensional inner-product spaces $\mathscr{U}$ and $\mathscr{V}$ over the field of real numbers (generalization to complex numbers is straightforward). The right-hand side $\mathfrak{B}$ represents an observation, or a collection of observations. When it is not contained within the range of the mapping, $\mathfrak{B} \notin \mathscr{R}(\mathcal{A})$, only an approximate solution can be constructed.

Vector (or single) and *matrix* (or multiple) *right-hand side* problems (1.1) have been studied for a long time; see especially [8], [41], [39], or [40] for the analysis and [30], [25], [32] for applications. *Tensor right-hand side* formulations typically originate in problems where $\mathcal{A}(\,\cdot\,)$ naturally outputs multidimensional data. This covers three-dimensional imaging problems, time-dependent two-dimensional problems, or models arising from linearization of problems depending on several parameters; see,

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[*] Received by the editors November 29, 2021; accepted for publication (in revised form) by J. L. Barlow September 13, 2022; published electronically February 2, 2023.
https://doi.org/10.1137/21M1462155

Funding: The work of the second and third authors was partially supported by the Technical University of Liberec (TUL) projects SGS-2021-4039, SGS-2022-4025.

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for example, [9], [30], [25], [32]. Problems with natural bilinear structure of the mapping $\mathcal{A}(\,\cdot\,)$ give rise to (1.1) with *bilinear models* and, typically, a matrix right-hand side; see [22], [23] for applications.

The individual linear approximation problems can be derived one from the other by subsequent generalization (downwards) or restriction (upwards) in the following way:

$$\begin{array}{lll}
\text{(i)} & Ax \approx b & \text{where}\quad A \in \mathbb{R}^{m\times n},\ x \in \mathbb{R}^{n},\ b \in \mathbb{R}^{m},\\
 & \updownarrow & \\
\text{(ii)} & AX \approx B & \text{where}\quad A \in \mathbb{R}^{m\times n},\ X \in \mathbb{R}^{n\times d},\ B \in \mathbb{R}^{m\times d},\\
 & \swarrow\!\!\!\!\!\nearrow \quad \nwarrow\!\!\!\!\!\searrow & \\
\text{(iii), (iv)} & A \times_1 \mathcal{X} \approx \mathcal{B},\ \ A_{\mathrm{L}} X A_{\mathrm{R}}^{\mathsf{T}} \approx B & \begin{cases} A \in \mathbb{R}^{m\times n},\ \mathcal{X} \in \mathbb{R}^{n\times d_2\times\cdots\times d_k},\ \mathcal{B} \in \mathbb{R}^{m\times d_2\times\cdots\times d_k},\\ A_{\mathrm{L}} \in \mathbb{R}^{m\times n}, A_{\mathrm{R}} \in \mathbb{R}^{d\times c},\ X \in \mathbb{R}^{n\times c},\ B \in \mathbb{R}^{m\times d},\end{cases}
\end{array}$$

where (i) and (ii) are the vector and matrix right-hand side problems, and (iv) has the bilinear model. In the tensor observation problem (iii), $\mathcal{B}, \mathcal{X}$ are k-way tensors and $\times_1$ stands for the standard 1-mode matrix-tensor product; see [21], [17], or (2.1).

1.1. The total least squares method. The principal difficulty with solving (1.1) is the presence of errors in the data that typically results in the observation $\mathfrak{B}$ not being contained in $\mathscr{R}(\mathcal{A})$. In order to find a meaningful approximate solution, we search for data corrections giving a modified compatible problem. To guarantee the optimality in some sense, selected minimality properties of the correction norms are prescribed, leading to methods widely known as *least squares techniques*. These include basic least squares (LS), total least squares (TLS), mixed LS-TLS, data LS, and regularized LS; see [10], [41] for an overview and references; see also [26] and [27]. Extending the basic LS from the case (i) to more general (ii)–(iv) is straightforward, since LS assumes errors only in the right-hand side and the constructed corrections of individual observations collected in B or $\mathcal{B}$ are independent; see [41]. However, this is not true for methods correcting both the model and the observation, as proved already in [8] for the widely used TLS. This complicates analysis and solution of TLS problems within (ii)–(iv).

For (i), TLS has been studied since the seventies; see [6], [4], [8], [36], [41]. It can be formulated here as

$$\min \|[g, E]\| \quad \text{subject to} \quad b + g \in \mathscr{R}(A + E), \tag{1.2}$$

where $\mathscr{R}(\cdot)$ is the matrix range. Equivalently, TLS searches for x_* such that $(A + E)\,x_* = b + g$. The norm here and throughout the paper refers either to the *Euclidean norm of a vector*, the *Frobenius norm of a matrix*, or their generalization to tensors: the square root of the sum of squares of all tensor entries. Note that other norms can also be relevant; see for example [24] and [42] for the TLS with a general unitarily invariant norm. In the case (ii), TLS takes the form

$$\min \|[G, E]\| \quad \text{subject to} \quad \mathscr{R}(B + G) \subseteq \mathscr{R}(A + E). \tag{1.3}$$

Extensive analysis can be found in particular in the influential book [41]; see also [37], [38], [39], [40]. Problems with more than one solution were studied in [44], [45]; for an extension to the mixed LS-TLS minimization see [29]. The full analysis of TLS-solvability was given later in [47] and [14]; see also [42]. For some recently proposed novel approaches we refer the reader to randomized algorithms [46], [48], or quantum algorithms [43], [49]. The TLS theory for problems (iii)–(iv) has not been addressed in full generality yet. Results for (iii) show that it is not essentially different from (ii) from the TLS perspective; see [30], [25], [32], and also [17]. Some TLS analyses for (iv) can found in [22] and [23].

Note that formally (ii)–(iv) can be rewritten into single right-hand side problems using vectorization (see [21]). Denote by $\mathrm{vec}(X)$ a vector obtained by stacking the columns of the matrix X below each other. Similarly $\mathrm{vec}(\mathcal{X})$ stacks all 1-mode fibers of the tensor $\mathcal{X}$ (ordered in the inverse lexicographical order w.r.t. their multi-indices) in a long vector; see [21]. The linear mappings $\mathcal{A}(\,\cdot\,)$ in (ii)–(iv) have, respectively, the following structure,

$$I_d \otimes A, \quad I_{d_k} \otimes \cdots \otimes I_{d_2} \otimes A, \quad A_{\mathrm{R}} \otimes A_{\mathrm{L}}, \tag{1.4}$$

where I_ℓ are ℓ-by-ℓ identity matrices and $\otimes$ is the Kronecker product; see [21]. The matrices in (1.4) are then multiplied by $\mathrm{vec}(X)$ in (ii) and (iv), or $\mathrm{vec}(\mathcal{X})$ in (iii). This reveals how the structure of the search set for the correction $\mathcal{E}(\,\cdot\,)$ is restricted to the given structure of the mapping $\mathcal{A}(\,\cdot\,)$ in TLS. Clearly, $\mathcal{E}(\,\cdot\,)$ has the form

$$I_d \otimes E, \qquad I_{d_k} \otimes \cdots \otimes I_{d_2} \otimes E$$

in (ii)–(iii), respectively. Although we search for E in all of $\mathbb{R}^{m\times n}$, from the perspective of the abstract setting (1.1), only a *proper subspace* of $\mathscr{L}(\mathscr{U},\mathscr{V})$ is involved. Similarly, the correction $(E_{\mathrm{L}}, E_{\mathrm{R}})$ of the pair of matrices $(A_{\mathrm{L}}, A_{\mathrm{R}})$ in (iv) is sought in the whole $\mathbb{R}^{m\times n} \times \mathbb{R}^{d\times c}$. The corresponding mapping correction, however, takes the form

$$(A_{\mathrm{R}} \otimes E_{\mathrm{L}}) + (E_{\mathrm{R}} \otimes A_{\mathrm{L}}) + (E_{\mathrm{R}} \otimes E_{\mathrm{L}}),$$

i.e., it lives within a *proper submanifold* of $\mathscr{L}(\mathscr{U},\mathscr{V})$. This gives another viewpoint on difficulties related to extending TLS to more general problems; see [17] and [18] for more details.

1.2. The fundamental core reduction.

In addition, it is well known [8] that even the simplest TLS minimization problem (1.2) may not have a solution for the given data. Besides the nontrivial solvability analysis referred to previously, an important original contribution to this area is represented by a series of papers [26], [27], [28]. Here the authors introduce the so-called core problem concept for problems (i). They prove, that there always exists a subproblem $A_{11}x_1 \approx b_1$ called the core problem within $Ax \approx b$ that contains *all the necessary and only the sufficient information* for solving the original problem. The core problem can be revealed by a specific orthogonal (SVD-based) transformation and has a lot of interesting properties. In particular, it always has a unique TLS solution. Moreover, after its back-transformation we get either the TLS solution of the original problem (if it exists) or the so-called nongeneric solution defined in [41] (if the TLS solution does not exist), both minimal in the norm; see [28]. Consequently, the core problem concept significantly simplifies and clarifies the TLS theory in the case (i). Furthermore, the core reduction can also be achieved iteratively by a well-known Krylov subspace procedure: the Golub–Kahan (sometimes also called Golub–Kahan–Lanczos) iterative bidiagonalization [5], as proved in [28]. Note that there are also other relevant ways of extracting the core problem, e.g., by employing randomized algorithms in the context of ill-posed data; see [48].

This fundamental data reducing concept was generalized to (ii) in a series of papers [15], [16], [13], giving the definition of the core problem, the SVD-based core reduction, the iterative scheme based on the band generalization of the Golub–Kahan iterative bidiagonalization, and finally basic results relating the structure of the core problem to the classification with respect to the TLS solvability. Recently, the core problem definition and the SVD-based core reduction have also been extended to (iii) and (iv); see [17], [18]. An iterative scheme for core reduction in the cases (iii) and (iv) has not been introduced yet.

1.3. Content and contribution of this work. In this paper, we unify and generalize the problems (i)–(iv) under a k-linear approximation problem with a tensor right-hand side. We extend the core reduction to this problem and describe the core problem properties (in particular the defining minimality conditions); see section 2. We briefly recapitulate how the Golub–Kahan iterative bidiagonalization and its band generalization provide core reduction for problems (i) and (ii); see section 3. Then, we show that the band bidiagonalization running k-times in parallel reveals the core problem within any k-linear approximation problem (including (iii) and (iv)); see section 4. The proof of the minimality is provided in section 5. Further properties of core problems extending previous results on basic approximation problems (i)–(ii) are analyzed.

Note that we strictly assume the exact arithmetic. Our goal is to demonstrate that it is in principle possible to reduce maximally the given data by an iterative core reduction provided by a generalized Golub–Kahan bidiagonalization. Computational aspects of the considered method must also be studied. However, they are beyond the scope of this analytical work.

2. Core problem within general multilinear approximation problem. First, we introduce a unifying multilinear approximation problem. Then, the core transformation for (i)–(iv) and its properties will be summarized. Finally, we extend the results to the multilinear case.

Let us start with the basic tensor-related notation adopted from the review paper [21]; see also [2], [20], [19]. Let $A_s = (a_{i,j}) \in \mathbb{R}^{m_s \times n_s}$ be a matrix and $\mathcal{X} = (x_{i_1,i_2,\ldots,i_k}) \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_k}$ a k-way tensor. The s-mode matrix-tensor product $A_s \times_s \mathcal{X}$ is defined entrywise as

$$(A_s \times_s \mathcal{X})_{i_1,\ldots,i_{s-1},i,i_{s+1},\ldots,i_k} = \sum_{\ell=1}^{n_s} a_{i,\ell} \cdot x_{i_1,\ldots,i_{s-1},\ell,i_{s+1},\ldots,i_k} \,. \tag{2.1}$$

As a shorthand for the multiplication of $\mathcal{X}$ by several matrices A_s, $s = 1, 2, \ldots, k$, in all the different modes (so called multilinear transformation of $\mathcal{X}$), we use

$$(A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) = A_1 \times_1 (A_2 \times_2 (\cdots \times_{k-1} (A_k \times_k \mathcal{X}) \cdots)). \tag{2.2}$$

The s-mode matricization of $\mathcal{X}$ refers to a matrix $\mathcal{X}^{\{s\}} \in \mathbb{R}^{n_s \times (\Delta/n_s)}$, where $\Delta \equiv \prod_{\ell=1}^{k} n_\ell$, that collects all the s-mode fibers (columns for $s = 1$, rows for $s = 2$, etc.) of $\mathcal{X}$ as columns in the inverse lexicographical order with respect to their multi-indices. Then (2.1) can be rewritten by using the standard matrix multiplication as

$$(A_s \times_s \mathcal{X})^{\{s\}} = A_s \mathcal{X}^{\{s\}}. \tag{2.3}$$

The vectorization of $\mathcal{X}$ similarly refers to a vector $\mathrm{vec}(\mathcal{X}) \in \mathbb{R}^{\Delta}$ that collects all the entries of $\mathcal{X}$ in the inverse lexicographical order with respect to their multi-indices. By employing the vectorization, (2.2) can be rewritten as

$$\mathrm{vec}(A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) = (A_k \otimes \cdots \otimes A_2 \otimes A_1)\, \mathrm{vec}(\mathcal{X}); \tag{2.4}$$

compare with (1.4).

2.1. *k*-linear approximation problem and TLS. Consider the k-linear approximation problem with a tensor right-hand side

$$\text{(v)}\; (A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) \approx \mathcal{B}, \quad \text{where} \quad \left\{ \begin{array}{l} A_s \in \mathbb{R}^{m_s \times n_s} \quad \text{for } s = 1, 2, \ldots, k, \\ \mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_k},\ \mathcal{B} \in \mathbb{R}^{m_1 \times m_2 \times \cdots \times m_k}. \end{array} \right.$$

Clearly, (v) covers all the previous formulations (i)–(iv) as special cases. For $A_2 = I, \ldots, A_k = I$ the k-linear problem reduces to $A_1 \times_1 \mathcal{X} \approx \mathcal{B}$. On the other hand, for $k = 2$ it reduces to $(A_1, A_2 \,|\, \mathcal{X}) \approx \mathcal{B}$, where $\mathcal{X}$ and $\mathcal{B}$ are tensor of order two (matrices), and

$$\operatorname{vec}(A_1, A_2 \,|\, \mathcal{X}) = (A_2 \otimes A_1) \operatorname{vec}(\mathcal{X}) = \operatorname{vec}(A_1\, \mathcal{X}\, A_2^{\mathsf{T}}).$$

The TLS minimization problem can be defined for (v) as

$$\min \left(\|\mathcal{G}\|^2 + \sum_{s=1}^{k} \|E_s\|^2 \right)^{\frac{1}{2}} \quad \text{s.t.} \quad \exists \mathcal{X}_* \,:\, (A_1 + E_1, A_2 + E_2, \ldots, A_k + E_k \,|\, \mathcal{X}_*) = \mathcal{B} + \mathcal{G};$$

i.e., in cases (iii) and (iv) corrections only to $(A, \mathcal{B})$ and $(A_{\mathrm{L}}, A_{\mathrm{R}}, B)$ are considered. Now we aim to generalize core reduction to (v).

2.2. Core revealing transformation for (i)–(iv). The core revealing transformation (CRT) for (i)–(iv) is realized by orthogonal matrices that we denote P, Q, M (possibly with subindices $M_2, \ldots, M_k$), and K. In paticular, in [28] it was shown that $\forall (A, b)$, $\exists (P, Q)$:

$$Ax \approx b \quad \xrightarrow{\text{CRT}} \quad \underbrace{(P^{\mathsf{T}} A Q)}_{A'} \underbrace{(Q^{\mathsf{T}} x)}_{x'} \approx \underbrace{(P^{\mathsf{T}} b)}_{b'}$$

and the transformed problem is block-structured as follows:

$$A'x' = \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \approx \begin{bmatrix} b_1 \\ 0 \end{bmatrix} = b'. \tag{2.5}$$

The original problem is therefore split into two subproblems

$$A_{11} x_1 \approx b_1 \qquad \text{and} \qquad A_{22} x_2 \approx 0,$$

where only the first one needs to be solved (as, trivially, $x_2 = 0$). If the first subproblem has *minimal dimensions* (over all such block-structure revealing orthogonal transformations), it is called the core problem. Such a minimally dimensioned subproblem always exists, as shown in [28]. Note that the transformation may exist in a degenerated (or trivial) form while yielding formally an empty matrix A_{22} with no rows or no columns in some cases.

In [15], it was similarly shown for (ii) that $\forall (A, B)$, $\exists (P, Q, M)$:

$$AX \approx B \quad \xrightarrow{\text{CRT}} \quad (P^{\mathsf{T}} A Q)(Q^{\mathsf{T}} X M) \approx (P^{\mathsf{T}} B M)$$

and

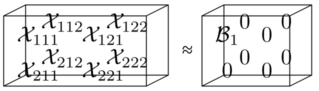
$$\begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \approx \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{2.6}$$

The problem (iii) was analyzed in [17] giving that $\forall(A,\mathcal{B})$, $\exists(P,Q,M_2,\dots,M_k)$:

$$A \times_1 \mathcal{X} \approx \mathcal{B} \quad \xrightarrow{\text{CRT}} \quad (P^{\mathsf{T}} A Q) \times_1 (Q^{\mathsf{T}}, M_2^{\mathsf{T}}, \dots, M_k^{\mathsf{T}} \,|\, \mathcal{X}) \approx (P^{\mathsf{T}}, M_2^{\mathsf{T}}, \dots, M_k^{\mathsf{T}} \,|\, \mathcal{B})$$

and (illustrated for $k = 3$)

(2.7) $$\begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \times_1$$



Finally, [18] derived for (iv) that $\forall(A_{\mathrm{L}}, A_{\mathrm{R}}, B)$, $\exists(P,Q,M,K)$:

$$A_{\mathrm{L}} X A_{\mathrm{R}}^{\mathsf{T}} \approx B \quad \xrightarrow{\text{CRT}} \quad (P^{\mathsf{T}} A_{\mathrm{L}} Q)(Q^{\mathsf{T}} X M)(M^{\mathsf{T}} A_{\mathrm{R}}^{\mathsf{T}} K) \approx (P^{\mathsf{T}} B K)$$

and

$$\begin{bmatrix} A_{\mathrm{L},11} & 0 \\ 0 & A_{\mathrm{L},22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} A_{\mathrm{R},11}^{\mathsf{T}} & 0 \\ 0 & A_{\mathrm{R},22}^{\mathsf{T}} \end{bmatrix} \approx \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{2.8}$$

Analogously to the case (i), the original problems (ii)–(iv) are split by these transformations into four, 2^k (eight in the above illustrated case), and four subproblems, respectively. Only the subproblem with the nonzero right-hand side has to be solved. If it has minimal dimensions, it is called the core problem. Consequently, core problems in the cases (i)–(iv) are subsequently

$$A_{11} x_1 \approx b_1, \qquad A_{11} X_{11} \approx B_1, \qquad A_{11} \times_1 \mathcal{X}_{11\dots1} \approx \mathcal{B}_1, \qquad A_{\mathrm{L},11} X_{11} A_{\mathrm{R},11}^{\mathsf{T}} \approx B_1.$$

2.3. Necessary and sufficient conditions for the minimality. First it would be useful to specify dimensions of individual objects in the core problems above. Let

$$A_{11},\, A_{\mathrm{L},11} \in \mathbb{R}^{\overline{m} \times \overline{n}}, \quad A_{\mathrm{R},11} \in \mathbb{R}^{\overline{d} \times \overline{c}}, \quad b_1 \in \mathbb{R}^{\overline{m}}, \quad B_1 \in \mathbb{R}^{\overline{m} \times \overline{d}}, \quad \mathcal{B}_1 \in \mathbb{R}^{\overline{m} \times \overline{d}_2 \times \cdots \times \overline{d}_k},$$

i.e., we use the same letters for the individual dimensions of core problems as for the original problems (see the schema in section 1), but overlined. For the core problems within (i)–(iii), we assume that

$$A_{11} \text{ has } \overline{\xi} \text{ distinct nonzero singular values with multiplicities } \overline{\mu}_i,\ i = 1, \dots, \overline{\xi},$$

and $\overline{\mu}_{\overline{\xi}+1} \equiv \dim(\mathscr{N}(A_{11}^{\mathsf{T}}))$, where $\mathscr{N}(\,\cdot\,)$ is the null-space. For the core problem within (iv), we similarly assume that

$$\begin{aligned} A_{\mathrm{L},11} &\text{ has } \overline{\xi} \text{ distinct nonzero singular values with multiplicities } \overline{\mu}_i,\ i = 1, \dots, \overline{\xi}, \\ A_{\mathrm{R},11} &\text{ has } \overline{\zeta} \text{ distinct nonzero singular values with multiplicities } \overline{\gamma}_j,\ j = 1, \dots, \overline{\zeta}, \end{aligned}$$

and $\overline{\mu}_{\overline{\xi}+1} \equiv \dim(\mathscr{N}(A_{\mathrm{L},11}^{\mathsf{T}}))$, and $\overline{\gamma}_{\overline{\zeta}+1} \equiv \dim(\mathscr{N}(A_{\mathrm{R},11}^{\mathsf{T}}))$ (note that one of the null-spaces may be trivial). Further, let

$$U_i \in \mathbb{R}^{\overline{m} \times \overline{\mu}_i}, \qquad U_{\mathrm{L},i} \in \mathbb{R}^{\overline{m} \times \overline{\mu}_i}, \quad \text{and} \quad U_{\mathrm{R},j} \in \mathbb{R}^{\overline{d} \times \overline{\gamma}_j}$$

be matrices having orthonormal bases of left singular vector subspaces of A_{11}, $A_{\mathrm{L},11}$, and $A_{\mathrm{R},11}$, respectively, as their columns, $i = 1, \dots, \overline{\xi}, \overline{\xi}+1$, $j = 1, \dots, \overline{\zeta}, \overline{\zeta}+1$.

Now we are ready to explore the core problem properties. We focus on the necessary and sufficient conditions for the minimality realized by a set of full column/row rank conditions; see [15]. We first show them for the matrix right-hand side problem (ii). Then we briefly discuss how they change for (i), (iii), and (iv). The full list of known properties can be found in the papers [28], [15], [16], [17], [18], and is summarized in Appendix A.

THEOREM 2.1. *Let* $AX \approx B$ *be a linear approximation problem and* $A_{11}X_{11} \approx B_1$ *a subproblem within, obtained by an orthogonal transformation yielding the block diagonal structure* (2.6)*. The subproblem has minimal dimensions (i.e., represents the core problem), if and only if the following three conditions are satisfied:*

(CP1) *The matrix* $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ *is of full column rank equal to* $\overline{n}$*.*
(CP2) *The matrix* $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$ *is of full column rank equal to* $\overline{d}$*.*
(CP3) *Matrices* $U_i^{\mathsf{T}} B_1 \in \mathbb{R}^{\overline{\mu}_i\times\overline{d}}$ *are of full row rank equal to* $\overline{\mu}_i$*,* $i = 1,\ldots,\overline{\xi},\overline{\xi}+1$*.*

For the proof, see [15, section 4.1].

Clearly, the problem (ii) becomes (i) when $d = 1$. Then for the core problem, $\overline{d} = 1$. Consequently the condition (CP2) is reduced to $b_1 \neq 0$ and (CP3) to $u_i^{\mathsf{T}} b_1 \neq 0$, where u_i are left singular vectors of A_{11}, $i = 1,\ldots,\overline{m}$ (while also implying $\overline{\xi} = \overline{m}$ and $\overline{\mu}_i = 1$ for all i); see [28].

The tensor right-hand side problem (iii) reduces back to (ii) for $k = 2$. Thus the matrices B and B_1 in the case (ii) can be seen as a tensor of the second order. In this sense

$$B_1^{\{1\}} = B_1 \quad \text{and} \quad B_1^{\{2\}} = B_1^{\mathsf{T}}.$$

Then (CP2) says that $B_1^{\{2\}} \in \mathbb{R}^{\overline{d}\times\overline{m}}$ is of full row rank and (CP3) says that $U_i^{\mathsf{T}} B_1^{\{1\}} \in \mathbb{R}^{\overline{\mu}_i\times\overline{d}}$ are of full row rank. To generalize (CP1)–(CP3) to (iii), i.e., to a tensor of the order k, only (CP2) needs to be modified to the following form: Matrices

$$\mathcal{B}_1^{\{s\}} \in \mathbb{R}^{\overline{d}_s\times(\Delta/\overline{d}_s)}, \qquad s = 2,\ldots,k,$$

are of *full row rank* equal to $\overline{d}_s$, here $\Delta \equiv \overline{m}\cdot\prod_{\ell=2}^{k}\overline{d}_\ell$; for more details see [17].

Finally, the problem (iv) reduces back to (ii) when $c = d$, $A_{\mathrm{L}} = A$, and $A_{\mathrm{R}} = I_d$, and analogously for the core problem within. From the SVD perspective, the case (ii) core problem is in fact the case (iv) core problem, where $A_{\mathrm{R},11} = I_{\overline{d}}$ has only one nonzero singular value with the multiplicity $\overline{d}$ and $\dim(\mathscr{N}(A_{\mathrm{R},11}^{\mathsf{T}})) = 0$. Thus $\overline{\zeta} = 1$, $\overline{\gamma}_1 = \overline{d}$, and $U_{\mathrm{R},1} = I_{\overline{d}}$, i.e.,

$$B_1 U_{\mathrm{R},1} = B_1.$$

To generalize (CP1)–(CP3) to (iv), i.e., to the bilinear problem, (CP1) needs to be extended so that both matrices $A_{\mathrm{L},11}$ and $A_{\mathrm{R},11}$ are of full column rank. (CP2) needs to be modified to the following form: Matrices

$$B_1 U_{\mathrm{R},j} \in \mathbb{R}^{\overline{m}\times\overline{\gamma}_j}, \qquad j = 1,\ldots,\overline{\zeta},\overline{\zeta}+1,$$

are of full column rank equal to $\overline{\gamma}_j$. In (CP3) we only formally replace matrices U_i by $U_{\mathrm{L},i}$; for more details see [18].

2.4. Extension to k-linear problems. Motivated by the previous derivations, we look for orthogonal matrices $P_s \in \mathbb{R}^{m_s\times m_s}$, $Q_s \in \mathbb{R}^{n_s\times n_s}$, $s = 1,2,\ldots,k$, realizing the orthogonal transformation of the multilinear problem (v) in the form

$$(A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) \approx \mathcal{B} \quad \xrightarrow{\text{CRT}}$$

$$\Big(\underbrace{P_1^{\mathsf{T}} A_1 Q_1}_{A'_1}, \underbrace{P_2^{\mathsf{T}} A_2 Q_2}_{A'_2}, \ldots, \underbrace{P_k^{\mathsf{T}} A_k Q_k}_{A'_k} \,\Big|\, \underbrace{(Q_1^{\mathsf{T}}, Q_2^{\mathsf{T}}, \ldots, Q_k^{\mathsf{T}} \,|\, \mathcal{X})}_{\mathcal{X}'}\Big) \approx \underbrace{(P_1^{\mathsf{T}}, P_2^{\mathsf{T}}, \ldots, P_k^{\mathsf{T}} \,|\, \mathcal{B})}_{\mathcal{B}'}$$

such that

$$\begin{aligned} A'_s &= \begin{bmatrix} A_{s,11} & 0 \\ 0 & A_{s,22} \end{bmatrix}, \quad A_{s,11} \in \mathbb{R}^{\overline{m}_s \times \overline{n}_s}, \quad s = 1, 2, \ldots, k, \\ \mathcal{B}' &= \operatorname{diag}_k(\mathcal{B}_1, 0), \quad \mathcal{B}_1 \in \mathbb{R}^{\overline{m}_1 \times \overline{m}_2 \times \cdots \times \overline{m}_k}. \end{aligned} \tag{2.9}$$

Here $\operatorname{diag}_k(\cdots)$ denotes a (block) diagonal tensor of order k with the arguments (treated also as kth order tensors) on its diagonal and the zero there represents a zero tensor of suitable dimensions, i.e., $0 \in \mathbb{R}^{(m_1 - \overline{m}_1) \times (m_2 - \overline{m}_2) \times \cdots \times (m_k - \overline{m}_k)}$. The original problem would then be split into 2^k subproblems

$$(A_{1,i_1 i_1}, A_{2,i_2 i_2}, \ldots, A_{k,i_k i_k} \,|\, \mathcal{X}_{i_1 i_2 \ldots i_k}) \approx \begin{cases} \mathcal{B}_1 & \text{if } i_1 = i_2 = \cdots = i_k = 1, \\ 0 & \text{otherwise,} \end{cases}$$

where $i_s \in \{1, 2\}$ for $s = 1, 2, \ldots, k$.

Since the k-linear approximation problem (v) represents a generalization of both (iii) and (iv), the core transformation can be constructed by combining strategies used for (iii) and (iv) in [17] and [18]. The basic steps are the following: The right-hand side preprocessing (used also in the iterative approach in section 4); the transformation of the system matrices A_s by employing their SVDs; the transformation of the right-hand side tensor; and the final permutation. Since the complete transformation, even in the cases (iii) and (iv), is very technical, we defer the description of our iterative procedure to section 4.

Now we provide the definition of the core problem.

DEFINITION 2.2 (core problem). *Let* $(A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) \approx \mathcal{B}$ *be a k-linear approximation problem and*

$$(A_{1,11}, A_{2,11}, \ldots, A_{k,11} \,|\, \mathcal{X}_{11\ldots1}) \approx \mathcal{B}_1 \tag{2.10}$$

a subproblem within, obtained by an orthogonal transformation yielding the block diagonal structure (2.9)*. If the subproblem has minimal dimensions, then we call it the core problem.*

In order to formulate a result generalizing Theorem 2.1, we introduce some SVD-related notation. We assume that

$$A_{s,11} \text{ has } \overline{\xi}_s \text{ distinct nonzero singular values with multiplicities } \overline{\mu}_{s,i_s}, \; i_s = 1, \ldots, \overline{\xi}_s,$$

and $\overline{\mu}_{s,\overline{\xi}_s+1} \equiv \dim(\mathscr{N}(A_{s,11}^{\mathsf{T}}))$ for $s = 1, 2, \ldots, k$ (note that $k-1$ of the null-spaces may be trivial). Further, let

$$U_{s,i_s} \in \mathbb{R}^{\overline{m}_s \times \overline{\mu}_{s,i_s}}, \qquad i_s = 1, \ldots, \overline{\xi}_s, \overline{\xi}_s + 1, \quad s = 1, 2, \ldots, k,$$

be matrices having orthonormal bases of left singular vector subspaces of $A_{s,11}$ as their columns. Now we formulate necessary and sufficient conditions for minimality.

THEOREM 2.3. *Let* $(A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) \approx \mathcal{B}$ *be a k-linear approximation problem and* $(A_{1,11}, A_{2,11}, \ldots, A_{k,11} \,|\, \mathcal{X}_{11\ldots1}) \approx \mathcal{B}_1$ *a subproblem within, obtained by an orthogonal transformation yielding the block diagonal structure* (2.9)*. The subproblem has* *minimal dimensions (i.e., represents the core problem), if and only if the following two conditions are satisfied:*

(CP1) *Matrices* $A_{s,11} \in \mathbb{R}^{\overline{m}_s \times \overline{n}_s}$ *are of full column rank equal to* $\overline{n}_s$*,* $s = 1, 2, \ldots, k$*.*

(CP2)–(CP3) *Matrices* $U_{s,i_s}^{\mathsf{T}} \mathcal{B}_1^{\{s\}} \in \mathbb{R}^{\overline{\mu}_{s,i_s} \times (\Delta / \overline{m}_s)}$ *are of full row rank equal to* $\overline{\mu}_{s,i_s}$*, where* $i_s = 1, 2, \ldots, \overline{\xi}_s, \overline{\xi}_s + 1$*,* $s = 1, 2, \ldots, k$*.*

Note that here $\Delta \equiv \prod_{\ell=1}^{k} \overline{m}_\ell$*.*

Note that any further orthogonal transformation of the subproblem (2.10) already satisfying (CP1) and (CP2)–(CP3) does not affect these properties, since they are orthogonally invariant. The proof for (v) is a generalization of the proofs for (i)–(iv). First, we show that there exists a transformation yielding the block-diagonal structure (2.9) determining the subproblem (2.10) satisfying the CP properties; see, in particular, [18, sections 3.1.1–3.1.3]. Then, we prove minimality of its dimensions; see [15, section 4.1].

Proof. Employing the full SVDs of the original matrices $A_s = U_s \Sigma_s V_s^{\mathsf{T}}$ allows us to write the approximation problem as

$$(U_1 \Sigma_1 V_1^{\mathsf{T}}, \ldots, U_k \Sigma_k V_k^{\mathsf{T}} \,|\, \mathcal{X}) \approx \mathcal{B},$$

i.e., after the vectorization and employing the mixed (Kronecker-matrix) product property

$$(U_k \otimes \cdots \otimes U_1)(\Sigma_k \otimes \cdots \otimes \Sigma_1)(V_k \otimes \cdots \otimes V_1)^{\mathsf{T}} \mathrm{vec}(\mathcal{X}) \approx \mathrm{vec}(\mathcal{B}).$$

This further gives an orthogonally transformed problem

$$(\Sigma_1, \ldots, \Sigma_k \,|\, \mathcal{Y}) \approx \mathcal{F}, \quad \text{where} \quad \mathcal{Y} = (V_1^{\mathsf{T}}, \ldots, V_k^{\mathsf{T}} \,|\, \mathcal{X}), \quad \mathcal{F} = (U_1^{\mathsf{T}}, \ldots, U_k^{\mathsf{T}} \,|\, \mathcal{B});$$

compare with [18, section 3.1.1].

Let A_s and thus also Σ_s have ξ_s distinct nonzero singular values with multiplicities μ_{s,i_s}, $i_s = 1, \ldots, \xi_s$, and let $\mu_{s,\xi_s+1} = \dim(\mathscr{N}(A_s^{\mathsf{T}}))$. Note that $\sum_{i_s=1}^{\xi_s+1} = m_s$. Then we partition the tensor $\mathcal{F}$ into a $(\xi_1 + 1) \times (\xi_2 + 1) \times \cdots \times (\xi_k + 1)$ grid of subtensors

$$\mathcal{F}_{i_1, i_2, \cdots, i_k} \in \mathbb{R}^{\mu_{1,i_1} \times \mu_{2,i_2} \times \cdots \times \mu_{k,i_k}}, \qquad i_s = 1, \ldots, \xi_s, \xi_s + 1, \quad s = 1, 2, \ldots, k.$$

Now we proceed with a joint Tucker-like decomposition of each of them. In particular, the matricization

$$\mathcal{F}^{\{s\}} \in \mathbb{R}^{m_s \times (\Delta / m_s)},$$

where $\Delta = \prod_{\ell=1}^{k} m_\ell$, is accordingly partitioned into $\xi_s + 1$ block-rows, with individual rows corresponding to the s-mode cofibers of $\mathcal{F}$. Let W_{s,i_s} be the orthogonal matrices of order μ_{s,i_s} with the left singular vectors obtained from the SVDs of the individual block-rows. Further, let

$$\begin{aligned} W_{s,\oplus} &= \mathrm{diag}(W_{s,1}, \ldots, W_{s,\xi_s}, W_{s,\xi_s+1}) \in \mathbb{R}^{m_s \times m_s}, \\ {W'}_{s,\oplus} &= \mathrm{diag}(W_{s,1}, \ldots, W_{s,\xi_s}, I_{n_s - \mathrm{rank}(A_s)}) \in \mathbb{R}^{n_s \times n_s}. \end{aligned}$$

Then

$$\mathcal{F}_{i_1, i_2, \cdots, i_k} = \Big(W_{1,i_1}, W_{2,i_2}, \ldots, W_{k,i_k} \,\Big|\, \mathrm{diag}_k(\mathcal{H}_{i_1, i_2, \cdots, i_k}, 0) \Big),$$

where

$$\mathcal{H}_{i_1,i_2,\cdots,i_k} \in \mathbb{R}^{\overline{\mu}_{1,i_1}\times\overline{\mu}_{2,i_2}\times\cdots\times\overline{\mu}_{k,i_k}}, \qquad \overline{\mu}_{s,i_s} \leq \mu_{s,i_s},$$

are, in fact, our joint-Tucker-like decompositions. This further leads to an orthogonally transformed problem

$$(\Sigma_1,\ldots,\Sigma_k \,|\, \mathcal{Z}) \approx \mathcal{H}, \quad \text{where} \quad \mathcal{Z} = (W_{1,\oplus}^{\mathsf{T}},\ldots,W'^{\mathsf{T}}_{k,\oplus} \,|\, \mathcal{Y}), \quad \mathcal{H} = (W_{1,\oplus}^{\mathsf{T}},\ldots,W_{k,\oplus}^{\mathsf{T}} \,|\, \mathcal{F}).$$

Since the matrices W_{s,i_s} are originated in the SVDs of block-rows, the first $\overline{\mu}_{s,i_s}$ rows in the i_sth block-row $\mathcal{H}^{\{s\}}$ are linearly independent; compare with [18, section 3.1.2].

The final step is the permutation, that collects all the blocks $\mathcal{H}_{i_1,i_2,\cdots,i_k}$ together in the leading principal corner of the tensor, while forming there $\mathcal{B}_1$. Application of this permutation to matrices Σ_s separates $A_{s,11}$ and $A_{s,22}$; compare with [18, section 3.1.3]. This separation can be done clearly such that all the zero columns of Σ_s stay as the last columns, and thus $A_{s,11}$ have linearly independent columns, i.e., (CP1) is satisfied. Moreover, the orthonormal bases of left singular vector subspaces of $A_{s,11}$ are formed by a Euclidean vector and thus (CP2)–(CP3) is satisfied by construction.

It remains to show the minimality. Consider another orthogonal transformation yielding the block-diagonal structure (2.9) with subproblems of dimensions

$$\widehat{A}_{s,11} \in \mathbb{R}^{\widehat{m}_s\times\widehat{n}_s}, \qquad \widehat{A}_{s,22} \in \mathbb{R}^{(m_s-\widehat{m}_s)\times(n_s-\widehat{n}_s)}, \qquad \widehat{\mathcal{B}}_1 \in \mathbb{R}^{\widehat{m}_1\times\widehat{m}_2\times\cdots\times\widehat{m}_k}.$$

Clearly, the transformed right-hand side always has zero projections into all left singular vector subspaces corresponding to the blocks $\widehat{A}_{s,22}$. Recall that we did the splitting in the first part of the proof by employing the SVDs of block-rows of the s-mode matricization of $\mathcal{F}$. Thus we minimize the number of nonzero rows in the corresponding matricization of $\mathcal{H}$ (because the number of nonzero rows is equal to the rank of the block-row) and maximize the number of zero rows. Thus singular values of $\widehat{A}_{s,22}$ form a subset of singular values of $A_{s,22}$. Consequently,

$$\operatorname{rank}(\widehat{A}_{s,11}) \geq \operatorname{rank}(A_{s,11}) = \overline{n}_s.$$

Therefore $\widehat{A}_{s,11}$ cannot have fewer columns (and smaller rank) than $\overline{n}_s$. Moreover, if $\widehat{A}_{s,11}$ contains some extra singular value in comparison to $A_{s,11}$, $\widehat{A}_{s,11}$ has larger dimensions then $A_{s,11}$ and the right-hand side has zero projection in the respective singular vector subspace, thus (CP2)–(CP3) is violated. If the multiplicity of some singular value in $\widehat{A}_{s,11}$ is larger then in $A_{s,11}$, then again $\widehat{A}_{s,11}$ has larger dimension then $A_{s,11}$ and the subproblem can be further transformed so that the right-hand side projection into the corresponding singular vector subspace contains zero s-mode cofibers (rows in the s-mode matricization). Thus again (CP2)–(CP3) is violated. ☐

Since the core problem is defined up to an orthogonal transformation, employing the SVD of $A_{s,11} = U_s[\begin{smallmatrix}\Sigma_s\\0\end{smallmatrix}]V_s^{\mathsf{T}}$, where Σ_s is square invertible (guaranteed by (CP1)), we can do the following transformation:

$$U_s^{\mathsf{T}}[\mathcal{B}_1^{\{s\}}, A_{s,11}]\,\operatorname{diag}(I, V_s) = U_s^{\mathsf{T}}[\mathcal{B}_1^{\{s\}}, A_{s,11}V_s] = \left[\begin{array}{c|c} \Phi & \Sigma_s \\ U^{\mathsf{T}}_{s,\overline{\xi}_s+1}\mathcal{B}_1^{\{s\}} & 0 \end{array}\right] \begin{array}{l} \}\overline{n}_s \\ \}\overline{m}_s - \overline{n}_s. \end{array}$$

This yields a block upper antitriangular matrix with full row rank blocks on the antidiagonal (Φ is an unimportant nonzero submatrix). The full row rank of the nonzero block of the last $m_s - n_s = \dim(\mathscr{N}(A_{s,11})) = \overline{\mu}_{s,\overline{\xi}_s+1} \geq 0$ rows is guaranteed by (CP2)–(CP3). Thus we obtain that:

(CP4) Matrices $[\mathcal{B}_1^{\{s\}}, A_{s,11}] \in \mathbb{R}^{\overline{m}_s \times (\overline{n}_s + \Delta/\overline{m}_s)}$ are of full row rank equal to $\overline{m}_s$, $s = 1, 2, \ldots, k$.

Compare this with analogous properties of problems (i)–(iv); cf. (CP4) in Appendix A.

3. Iterative core reduction for problems (i)–(ii).

The CRTs (2.5)–(2.8) and (2.9) can be constructed using the SVD and the Tucker decomposition, the high-order variant of the SVD; see [28], [15], [16]. The resulting core problems have nice structure (e.g., system matrices A_{11} are typically diagonal). However, calculation of the SVD and Tucker decompositions is computationally expensive. Core problems can also be obtained iteratively. We summarize the technique for problems (i)–(ii) and explain the influence of starting vectors.

3.1. Golub–Kahan bidiagonalization and its band generalization.

The core problem in the vector right-hand side case $Ax \approx b$ is reachable by the *Golub–Kahan* (GK) *iterative bidiagonalization* of A starting with the vector $b/\|b\|$; see [28]. For this three-term recurrence algorithm, the computation terminates when one of the two normalization coefficients computed in each iteration is zero. The system matrix A_{11} then has a bidiagonal form, e.g.,

$$A \xrightarrow{\text{GK}} A_{11} = \begin{bmatrix} \clubsuit & & & & \\ \clubsuit & \clubsuit & & & \\ & \clubsuit & \clubsuit & & \\ & & \clubsuit & \clubsuit & \\ & & & \clubsuit & \end{bmatrix} \boxed{0} \quad ,$$

where "♣" denotes nonzero entries (the other entries are zeros); boxed zero denotes the zero normalization coefficient.

In the matrix right-hand side case, the core problem is extracted by the *band generalization of GK* (BGGK) [7] of A. The iterations need to be started with an orthonormal basis of the range of B; see [1] and, in particular, [16] for a detailed explanation and description of the algorithm. BGGK produces a band diagonal matrix A_{11} with $\overline{d} = \operatorname{rank}(B_1) = \operatorname{rank}(B)$ diagonals. During the process the current width of the band is subsequently reduced as individual underlying Krylov subspaces become A-invariant. This effect is called the (upper or lower) deflation. After $\overline{d}$ deflations, the core problem is separated. The process can also be viewed as a *block generalization of GK*, where the nonzero entries in the standard GK are replaced by lower triangular matrices in the column echelon form (in the block-superdiagonal) and upper triangular matrices in the row echelon form (in the block subdiagonal). See an example with $\overline{d} = 4$:

$$A \xrightarrow{\text{BGGK}} A_{11} = \left[\begin{array}{cccc|cc|c} \clubsuit & & & & & & \\ \heartsuit & \clubsuit & & & & & \\ \heartsuit & \heartsuit & \clubsuit & & & & \\ \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & \\ \hline \clubsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & \\ & \boxed{0} & \clubsuit & \heartsuit & \heartsuit & \boxed{0} & \\ & & & \clubsuit & \heartsuit & \clubsuit & \\ \hline & & & & \clubsuit & \heartsuit & \clubsuit \\ \hline & & & & & \boxed{0} & \clubsuit \end{array}\right] \boxed{0} \quad ,$$

where "♡" denotes entries that may be zero as well as nonzero; boxed zeros denote the individual deflations. The vertical and horizontal lines separate the individual blocks computed in the iterates of the block algorithm.

3.2. Impact of choice of starting vectors. In the case (i), GK iteratively (column-by-column) builds up the matrices P and Q from (2.5). The first column of P is the starting vector $p_1 = b/\gamma_1$, where $\gamma_1 = \|b\|$. The first column of Q is $q_1 = A^{\mathsf{T}} p_1/\alpha_1$, where $\alpha_1 = \|A^{\mathsf{T}} p_1\|$. Then the process continues as

$$p_j\gamma_j \leftarrow Aq_{j-1} - p_{j-1}\alpha_{j-1}, \qquad \|p_j\| = 1,\ \gamma_j \geq 0, \tag{3.1}$$

$$q_j\alpha_j \leftarrow A^{\mathsf{T}} p_j - q_{j-1}, \qquad \|q_j\| = 1,\ \alpha_j \geq 0, \tag{3.2}$$

for $j = 2, 3, \ldots$ till separating the core problem. The remaining columns of P and Q can be chosen arbitrarily such that P and Q are square orthogonal (for determination of the core problem they are in fact not needed). Then

$$P^{\mathsf{T}}[b, A]\,\mathrm{diag}(1, Q) = \left[\begin{array}{c||c} \|b\| & \\ 0 & \\ \vdots & P^{\mathsf{T}}AQ \\ 0 & \end{array}\right] = \left[\begin{array}{c||cccc} \gamma_1 & \alpha_1 & & & \\ & \gamma_2 & \alpha_2 & & \\ & & \gamma_3 & \ddots & \\ & & & \ddots & \end{array}\right],$$

giving schematically the structure of core data (2.5):

$$[b, A] \quad \xrightarrow{\text{GK}} \quad [b_1, A_{11}] = \left[\begin{array}{c||cccc} \clubsuit & \clubsuit & & & \\ & \clubsuit & \clubsuit & & \\ & & \clubsuit & \clubsuit & \\ & & & \clubsuit & \clubsuit \\ & & & & \clubsuit \end{array}\right].$$

For problems (ii) with B of full column rank Björck [1] proposed to use the basis of $\mathscr{R}(B)$ obtained by the thin QR decomposition of B as the starting set of vectors for BGGK. This concept can be simply generalized to any $B \in \mathbb{R}^{m\times d}$, $\overline{d} = \mathrm{rank}(B)$, by employing two subsequent QR's. In particular, in [16] it is proposed to do first the full LQ decomposition of B (the full QR decompostion of B^{T}) to get the orthogonal matrix M (see (2.6)). Thus

$$B = LM^{\mathsf{T}} = [L', 0]M^{\mathsf{T}}, \qquad \text{where} \qquad M^{-1} = M^{\mathsf{T}} \in \mathbb{R}^{d\times d} \quad \text{and} \quad L' \in \mathbb{R}^{m\times \overline{d}},$$

is a full column rank matrix in the lower triangular column echelon form. Then the approach of Björck can be applied to L'. The thin QR decomposition yields

$$L' = P_{1:\overline{d}}\Gamma, \qquad \text{where} \qquad P_{1:\overline{d}} \in \mathbb{R}^{m\times \overline{d}}, \quad P_{1:\overline{d}}^{\mathsf{T}} P_{1:\overline{d}} = I_{\overline{d}}, \quad \text{and} \quad \Gamma \in \mathbb{R}^{\overline{d}\times \overline{d}},$$

is square invertible in the upper triangular form. The $\overline{d}$ columns of $P_{1:\overline{d}}$ then form the orthonormal basis of $\mathscr{R}(B)$ used for starting BGGK. Altogether we have

$$B = P_{1:\overline{d}}\,[\Gamma, 0]M^{\mathsf{T}} \qquad \text{and} \qquad P^{\mathsf{T}}[B, A]\,\mathrm{diag}(M, Q) = \left[\begin{array}{cc||c} \Gamma & 0 & \\ 0 & 0 & P^{\mathsf{T}}AQ \end{array}\right],$$

giving schematically the structure of core data (2.6), e.g.:

$$[B, A] \quad \xrightarrow{\text{BGGK}} \quad [B_1, A_{11}] = \left[\begin{array}{cccc||ccccccc}
\clubsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & & & & \\
 & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & & & \\
 & & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & & \\
 & & & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & \\
 & & & & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & \\
 & & & & & \boxed{0} & \clubsuit & \heartsuit & \heartsuit & \boxed{0} & \\
 & & & & & & & \clubsuit & \heartsuit & \clubsuit & \\
 & & & & & & & & \clubsuit & \heartsuit & \clubsuit \\
 & & & & & & & & & \boxed{0} & \clubsuit
\end{array}\right].$$

Note that the first full LQ decomposition is in [15], [16], [17] called the *right-hand side preprocessing* since it precedes the main iterative part of BGGK, while yielding the nice band-diagonal shape of the resulting problem $[B_1, A_{11}]$. However, since the matrix multiplication is associative, it does not need to be done as the first step.

On the other hand, the actions of the involved algorithms are not commutative. Starting with the thin QR decomposition of B, $B = \widetilde{P}_{1:\overline{d}}\widetilde{U}$, we get in general another basis of $\mathscr{R}(B)$ and a full row rank upper triangular $\widetilde{U}$ in row echelon form. The subsequent *LQ* decomposition of $\widetilde{U}$ gives $\widetilde{U} = [\widetilde{\Gamma}, 0]\widetilde{M}^{\mathsf{T}}$ and can be done ex-post as postprocessing. The main difference of the "tilded" decomposition $B = \widetilde{P}_{1:\overline{d}}[\widetilde{\Gamma}, 0]\widetilde{M}^{\mathsf{T}}$ is that Γ is an upper but $\widetilde{\Gamma}$ is a lower triangular invertible matrix (decompositions of B in these two forms are also traditionally called the URV$^{\mathrm{T}}$ and ULV$^{\mathrm{T}}$ decompositions; see [3], [11], [31]). Then, for example:

$$[B, A] \quad \xrightarrow{\text{BGGK}} \quad [B_1, A_{11}] = \left[\begin{array}{cccc||ccccccc}
\clubsuit & & & & \clubsuit & & & & & & \\
\heartsuit & \clubsuit & & & \heartsuit & \clubsuit & & & & & \\
\heartsuit & \heartsuit & \clubsuit & & \heartsuit & \heartsuit & \boxed{0} & & & & \\
\heartsuit & \heartsuit & \heartsuit & \clubsuit & \heartsuit & \heartsuit & \clubsuit & & & & \\
 & & & & \clubsuit & \heartsuit & \heartsuit & \clubsuit & & & \\
 & & & & & \clubsuit & \heartsuit & \heartsuit & \clubsuit & & \\
 & & & & & & \boxed{0} & \boxed{0} & \clubsuit & \clubsuit & \\
 & & & & & & & & & \clubsuit & \clubsuit \\
 & & & & & & & & & & \clubsuit
\end{array}\right].$$

In general, any basis $\widehat{P}_{1:\overline{d}}$ of $\mathscr{R}(B)$ can be used for starting BGGK, and any decomposition of the form $B = \widehat{P}_{1:\overline{d}}[\widehat{\Gamma}, 0]\widehat{M^{\mathsf{T}}}$, where $\widehat{\Gamma}$ is square invertible, can used for the same purpose. A subsequent QR or LQ decomposition of $\widehat{\Gamma}$ again yields a decomposition of B in the URV$^{\mathrm{T}}$ or ULV$^{\mathrm{T}}$ form, respectively. Naturally, also the SVD of B can be used, but this would result in higher computational cost.

Note that a different set of starting vectors (different orthonormal basis of $\mathscr{R}(B)$) can drive BGGK for the given fixed $[B, A]$ into differently shaped $[B_1, A_{11}]$, since deflations may occur in different iterations. However, from the conditions (CP1)–(CP3) it follows that the final dimensions of the core data $A_{11} \in \mathbb{R}^{\overline{m} \times \overline{n}}$ and $B_1 \in \mathbb{R}^{\overline{m} \times \overline{d}}$ are independent of the choice of the starting set. Consequently, the same holds for the total number of upper and lower deflations

$$\#\,\text{upper def's} = \overline{m} - \overline{n} \qquad \text{and} \qquad \#\,\text{lower def's} = (\overline{n} + \overline{d}) - \overline{m};$$

see [16] for details.

4. Iterative core reduction for problems (iii)–(v).

In this section we generalize BGGK to problems (iii)–(v). First note that for (iii) and (v), we have to preprocess a tensor right-hand side. For this purpose, we employ the standard Tucker decomposition; see [33], [34], [35]; see also [21].

Let $\mathcal{B} \in \mathbb{R}^{m_1 \times m_2 \times \cdots \times m_k}$ be a tensor of multilinear rank

$$\text{rank}(\mathcal{B}) = (r_1, r_2, \ldots, r_k), \qquad \text{i.e.,} \qquad r_j \equiv \text{rank}_j(\mathcal{B}) \equiv \text{rank}(\mathcal{B}^{\{j\}}) \tag{4.1}$$

for $j = 1, 2, \ldots, k$. Denote $\Delta = \prod_{\ell=1}^{k} m_\ell$ and consider the SVD of the jth matricization in the following form:

$$\mathcal{B}^{\{j\}} = U_j \Sigma_j V_j^{\mathsf{T}} \in \mathbb{R}^{m_j \times (\Delta/m_j)}, \quad U_j = [U'_j, U''_j] \in \mathbb{R}^{m_j \times m_j}, \quad U'_j \in \mathbb{R}^{m_j \times r_j}. \tag{4.2}$$

Then

$$\mathcal{B}_{\text{TC}} \equiv (U'^{\mathsf{T}}_1, U'^{\mathsf{T}}_2, \ldots, U'^{\mathsf{T}}_k \,|\, \mathcal{B}) \in \mathbb{R}^{r_1 \times r_2 \times \cdots \times r_k} \tag{4.3}$$

is the so-called *Tucker core* of the tensor $\mathcal{B}$ (the terminology is not related to the core problem terminology in this paper) and

$$\mathcal{B} = (U'_1, U'_2, \ldots, U'_k \,|\, \mathcal{B}_{\text{TC}}) = \Big(U_1, U_2, \ldots, U_k \,|\, \text{diag}_k(\mathcal{B}_{\text{TC}}, 0)\Big) \tag{4.4}$$

are the economic and full *Tucker decompositions* of $\mathcal{B}$, respectively. Alternatively other variants of the Tucker decomposition then the SVD based can be used. We mention this in the last subsection.

4.1. BGGK for tensor right-hand side problems.

We are looking for an iterative BGGK-based process such that

$$A \times_1 \mathcal{X} \approx \mathcal{B} \qquad \text{reduces to} \qquad A_{11} \times_1 \mathcal{X}_{11\ldots1} \approx \mathcal{B}_1.$$

The matricization of $A \times_1 \mathcal{X} \approx \mathcal{B}$ transforms the problem into a matrix right-hand side one

$$A\mathcal{X}^{\{1\}} \approx \mathcal{B}^{\{1\}}.$$

The CRT thus becomes the transformation for the problem (ii), however, with an additional constraint. In particular,

$$(P^{\mathsf{T}} A Q)(Q^{\mathsf{T}} \mathcal{X}^{\{1\}} M) \approx (P^{\mathsf{T}} \mathcal{B}^{\{1\}} M) \qquad \text{with} \qquad M \equiv M_k \otimes \cdots \otimes M_2,$$

i.e., M is a Kronecker product with orthogonal factors; see [17, eq. (6.4)].

To find it, we start with the Tucker decomposition (4.1)–(4.4) of $\mathcal{B} \in \mathbb{R}^{m \times d_2 \times \cdots \times d_k}$. We need to link the individual objects in the decomposition to the orthogonal transformation (2.7). First,

$$P_{1:r_1} \equiv U'_1 \in \mathbb{R}^{m \times r_1}, \qquad r_1 = \text{rank}(\mathcal{B}^{\{1\}})$$

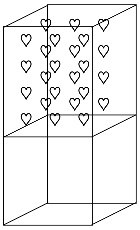
play the role of the starting vectors of BGGK and form the first part of the orthogonal transformation matrix P. Then,

$$M_j \equiv U_j = [U'_j, U''_j] \in \mathbb{R}^{d_j \times d_j}, \quad U'_j \in \mathbb{R}^{d_j \times \overline{d}_j}, \quad \overline{d}_j \equiv r_j = \text{rank}(\mathcal{B}^{\{j\}}), \qquad j = 2, \ldots, k,$$

are the other right-hand side transformation matrices, where $\overline{d}_j$ denote the latter dimensions of $\mathcal{B}_1$, $j = 2, \ldots, k$; see core problem properties in section 2.3 or Appendix A. The Tucker core $\mathcal{B}_{\text{TC}} \in \mathbb{R}^{r_1 \times \overline{d}_2 \times \cdots \times \overline{d}_k}$ of $\mathcal{B}$ forms the main (nonzero) part of $\mathcal{B}_1$.

Having orthonormal starting vectors $P_{1:r_1} \equiv U'_1$, we can now run BGGK as in the previous section to get (2.7). Schematically, e.g., for $k = 3$ and $r_1 = 4$

(4.5) $(\mathcal{B}, A) \xrightarrow{\text{BGGK}} (\mathcal{B}_1, A_{11}) = \Bigg($



$$, \left[\begin{array}{cccc} \clubsuit & & & \\ \heartsuit & \clubsuit & & \\ \heartsuit & \heartsuit & & \\ \heartsuit & \heartsuit & \clubsuit & \\ \hline \clubsuit & \heartsuit & \heartsuit & \clubsuit \\ & \clubsuit & \heartsuit & \heartsuit \\ & & \clubsuit & \heartsuit \end{array}\right] \Bigg).$$

Here the upper $4 \times 3 \times 2$ part of the tensor $\mathcal{B}_1$ (filled with hearts) is the (full multilinear rank) Tucker core $\mathcal{B}_{\text{TC}}$ of the original $\mathcal{B}$, concatenated in the first mode by a zero block of appropriate size; $0 \in \mathbb{R}^{(\overline{m}-r_1) \times \overline{d}_2 \times \cdots \times \overline{d}_k}$ in general. After a vectorization the core problem takes the form

$$[\mathcal{B}_1^{\{1\}}, A_{11}] = \left[\begin{array}{ccc|ccc||cccc} \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & \\ \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & \\ \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & & \\ \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & \\ \hline & & & & & & \clubsuit & \heartsuit & \heartsuit & \clubsuit \\ & & & & & & & \clubsuit & \heartsuit & \heartsuit \\ & & & & & & & & \clubsuit & \heartsuit \end{array}\right], \tag{4.6}$$

where the first vertical line separates the individual frontal slices of $\mathcal{B}_1$. Note that applying BGGK directly to $[\mathcal{B}^{\{1\}}, A]$ would yield the full column rank right-hand side B_1, representing a factor of $\mathcal{B}_1^{\{1\}} = B_1 \widehat{M}^{\mathsf{T}}$ for some $\widehat{M} \in \mathbb{R}^{(\prod_{\ell=2}^{k} \overline{d}_\ell) \times r_1}$, $\widehat{M}^{\mathsf{T}} \widehat{M} = I_{r_1}$.

4.2. BGGK for bilinear problems with a matrix right-hand side.

In case (iv) the whole setup is different. The linear mapping is represented by two matrices and we are looking for a process such that

$$A_{\text{L}} X A_{\text{R}}^{\mathsf{T}} \approx B \qquad \text{reduces to} \qquad A_{\text{L},11} X_{11} A_{\text{R},11}^{\mathsf{T}} \approx B_1.$$

We now show that this can be achieved via appropriate preprocessing of B followed by two independent BGGK processes for A_{L} and A_{R}, respectively. Even though the derivations are based on Householder reflection matrices, computation of BGGK iterates can be realized by band (block) tridiagonalization using the well-known equivalence of these approaches; see section 3.1.

We start with the SVD of the right-hand side. Let $\text{rank}(B) = r$ and $B = U \Sigma V^{\mathsf{T}} \in \mathbb{R}^{m \times d}$ with the partitioning

$$U = [U', U''] \in \mathbb{R}^{m \times m}, \quad U' \in \mathbb{R}^{m \times r}, \quad V = [V', V''] \in \mathbb{R}^{d \times d}, \quad V' \in \mathbb{R}^{d \times r}, \tag{4.7}$$

and $\Sigma = \text{diag}(\Sigma', 0)$, where $\Sigma' \in \mathbb{R}^{r \times r}$ is square, diagonal, and invertible. Consider the extended data matrix

$$\begin{bmatrix} B & A_{\text{L}} \\ A_{\text{R}}^{\mathsf{T}} & 0 \end{bmatrix} \in \mathbb{R}^{(c+m) \times (n+d)} \tag{4.8}$$

and apply the following transformation

$$\operatorname{diag}(U, I_c)^{\mathsf{T}} \begin{bmatrix} B & A_{\mathrm{L}} \\ A_{\mathrm{R}}^{\mathsf{T}} & 0 \end{bmatrix} \operatorname{diag}(V, I_n) = \begin{bmatrix} \Sigma' & 0 & U'^{\mathsf{T}} A_{\mathrm{L}} \\ 0 & 0 & U''^{\mathsf{T}} A_{\mathrm{L}} \\ (V'^{\mathsf{T}} A_{\mathrm{R}})^{\mathsf{T}} & (V''^{\mathsf{T}} A_{\mathrm{R}})^{\mathsf{T}} & 0 \end{bmatrix}. \tag{4.9}$$

This block structure is particularly advantageous, since it now allows us to treat the two parts involving A_{L} and A_{R} independently.

To transform the part of (4.9) corresponding to A_{L}, we first find a Householder matrix $H_{\mathrm{L},1}$ such that the first row of

$$(U'^{\mathsf{T}} A_{\mathrm{L}}) H_{\mathrm{L},1} \qquad \text{and thus also} \qquad (U^{\mathsf{T}} A_{\mathrm{L}}) H_{\mathrm{L},1}$$

is zero except for the first entry. Then we apply a Householder matrix $H_{\mathrm{L},2}$ so that the same holds for the first column of

$$H_{\mathrm{L},2}^{\mathsf{T}} (U''^{\mathsf{T}} A_{\mathrm{L}} H_{\mathrm{L},1}).$$

Similarly, to transform the part of (4.9) corresponding to A_{R} we first apply a Householder matrix $H_{\mathrm{R},1}$ that zeros out the entries in the first row of

$$(V'^{\mathsf{T}} A_{\mathrm{R}}) H_{\mathrm{R},1} \qquad \text{and thus also} \qquad (V^{\mathsf{T}} A_{\mathrm{R}}) H_{\mathrm{R},1}$$

except for the first one. Then we apply a Householder matrix $H_{\mathrm{R},2}$ so that we get the same for the first column of

$$H_{\mathrm{R},2}^{\mathsf{T}} (V''^{\mathsf{T}} A_{\mathrm{R}} H_{\mathrm{R},1}).$$

The whole orthogonal transformation is then

$$\begin{aligned} &\begin{bmatrix} I_r & 0 & 0 \\ 0 & H_{\mathrm{L},2} & 0 \\ 0 & 0 & H_{\mathrm{R},1} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \Sigma' & 0 & U'^{\mathsf{T}} A_{\mathrm{L}} \\ 0 & 0 & U''^{\mathsf{T}} A_{\mathrm{L}} \\ (V'^{\mathsf{T}} A_{\mathrm{R}})^{\mathsf{T}} & (V''^{\mathsf{T}} A_{\mathrm{R}})^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} I_r & 0 & 0 \\ 0 & H_{\mathrm{R},2} & 0 \\ 0 & 0 & H_{\mathrm{L},1} \end{bmatrix} \\ &\qquad = \begin{bmatrix} \Sigma' & 0 & U'^{\mathsf{T}} A_{\mathrm{L}} H_{\mathrm{L},1} \\ 0 & 0 & H_{\mathrm{L},2}^{\mathsf{T}} U''^{\mathsf{T}} A_{\mathrm{L}} H_{\mathrm{L},1} \\ H_{\mathrm{R},1}^{\mathsf{T}} (V'^{\mathsf{T}} A_{\mathrm{R}})^{\mathsf{T}} & H_{\mathrm{R},1}^{\mathsf{T}} (V''^{\mathsf{T}} A_{\mathrm{R}})^{\mathsf{T}} H_{\mathrm{R},2} & 0 \end{bmatrix}. \end{aligned}$$

After several steps, the transformation matrices applied from the left and right have the forms

$$\begin{aligned} &\operatorname{diag}(I_r,\, H_{\mathrm{L},2} H_{\mathrm{L},4} H_{\mathrm{L},6} \cdots,\, H_{\mathrm{R},1} H_{\mathrm{R},3} H_{\mathrm{R},5} \cdots), \\ &\operatorname{diag}(I_r,\, H_{\mathrm{R},2} H_{\mathrm{R},4} H_{\mathrm{R},6} \cdots,\, H_{\mathrm{L},1} H_{\mathrm{L},3} H_{\mathrm{L},5} \cdots), \end{aligned} \tag{4.10}$$

respectively.

In summary, BGGK of the extended data matrix (4.8) splits equivalently into two independent BGGK processes. Schematically:

$$\begin{bmatrix} B & A_{\mathrm{L}} \\ A_{\mathrm{R}}^{\mathsf{T}} & 0 \end{bmatrix} \xrightarrow{\text{BGGK}} \begin{bmatrix} B_1 & A_{\mathrm{L},11} \\ A_{\mathrm{R},11}^{\mathsf{T}} & 0 \end{bmatrix}$$

is equivalent to

$$(4.11)\qquad \begin{array}{llll} [B, A_{\mathrm{L}}] & \xrightarrow{\text{BGGK}} [B_{\mathrm{L},1}, A_{\mathrm{L},11}], & \text{where} \quad B_1 = [B_{\mathrm{L},1}, 0] & \text{and} \\ [B^{\mathsf{T}}, A_{\mathrm{R}}] & \xrightarrow{\text{BGGK}} [B_{\mathrm{R},1}, A_{\mathrm{R},11}], & \text{where} \quad B_1 = \begin{bmatrix} B_{\mathrm{R},1}^{\mathsf{T}} \\ 0 \end{bmatrix}. & \end{array}$$

Note that B_1 computed for (4.8) has some extra zero rows and columns in comparison to the right-hand sides produced in separate processes (4.11); see the following example with $r = \mathrm{rank}(B) = 4$:

$$(4.12)\qquad \begin{bmatrix} B_1 & A_{\mathrm{L},11} \\ A_{\mathrm{R},11}^{\mathsf{T}} & 0 \end{bmatrix} = \left[\begin{array}{cccc|ccc||cccc} \clubsuit & & & & & & & \clubsuit & & & \\ & \clubsuit & & & & & & \heartsuit & \clubsuit & & \\ & & \clubsuit & & & & & \heartsuit & \heartsuit & & \\ & & & \clubsuit & & & & \heartsuit & \heartsuit & \clubsuit & \\ \hline & & & & & & & \clubsuit & \heartsuit & \heartsuit & \clubsuit \\ & & & & & & & & \clubsuit & \heartsuit & \heartsuit \\ & & & & & & & & & \clubsuit & \heartsuit \\ \hline\hline \clubsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & & & & \\ & & \clubsuit & \heartsuit & \heartsuit & \clubsuit & & & & & \\ & & & & \clubsuit & \heartsuit & \clubsuit & & & & \end{array}\right].$$

Further note that since we started with the SVD of B, the nonzero full rank block of B_1 is square diagonal and equal to Σ'. Different initial decompositions of B may result in different full rank blocks, but with the same singular values (see section 3.2).

It remains to specify the orthogonal transformation matrices in (2.8). Comparing

$$\begin{bmatrix} P^{\mathsf{T}} B K & P^{\mathsf{T}} A_{\mathrm{L}} Q \\ M^{\mathsf{T}} A_{\mathrm{R}}^{\mathsf{T}} K & 0 \end{bmatrix} = \begin{bmatrix} P & 0 \\ 0 & M \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} B & A_{\mathrm{L}} \\ A_{\mathrm{R}}^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} K & 0 \\ 0 & Q \end{bmatrix}$$

and (4.9) combined with (4.10) gives

$$\begin{bmatrix} P & 0 \\ 0 & M \end{bmatrix} = \begin{bmatrix} U' & U'' & 0 \\ 0 & 0 & I_d \end{bmatrix} \begin{bmatrix} I_r & 0 & 0 \\ 0 & H_{\mathrm{L},2} H_{\mathrm{L},4} H_{\mathrm{L},6} \cdots & 0 \\ 0 & 0 & H_{\mathrm{R},1} H_{\mathrm{R},3} H_{\mathrm{R},5} \cdots \end{bmatrix},$$

$$\begin{bmatrix} K & 0 \\ 0 & Q \end{bmatrix} = \begin{bmatrix} V' & V'' & 0 \\ 0 & 0 & I_n \end{bmatrix} \begin{bmatrix} I_r & 0 & 0 \\ 0 & H_{\mathrm{R},2} H_{\mathrm{R},4} H_{\mathrm{R},6} \cdots & 0 \\ 0 & 0 & H_{\mathrm{L},1} H_{\mathrm{L},3} H_{\mathrm{L},5} \cdots \end{bmatrix}.$$

Consequently, the starting vectors for the two independent BGGKs in (4.11) are

$$P_{1:r} = U' \qquad \text{and} \qquad K_{1:r} = V',$$

respectively.

4.3. BGGK for k-linear problems with a tensor right-hand side.

In the general k-linear case, we wish to design a process such that

$$(A_1, A_2, \ldots, A_k \,|\, \mathcal{X}) \approx \mathcal{B} \qquad \text{reduces to} \qquad (A_{1,11}, A_{2,11}, \ldots, A_{k,11} \,|\, \mathcal{X}_{11\ldots 1}) \approx \mathcal{B}_1.$$

This can be done by a straightforward combination of approaches from sections 4.1 and 4.2. We start with the Tucker decomposition of the tensor $\mathcal{B} \in \mathbb{R}^{m_1 \times m_2 \times \cdots \times m_k}$, as in section 4.1. Let

$$\operatorname{rank}(\mathcal{B}) = (r_1, r_2, \ldots, r_k) \qquad \text{and} \qquad \mathcal{B} = (U'_1, U'_2, \ldots, U'_k \,|\, \mathcal{B}_{\mathrm{TC}})$$

(see (4.1)–(4.4)), i.e., the columns of $U'_s \in \mathbb{R}^{m_s \times r_s}$ represent an orthonormal basis of $\mathscr{R}(\mathcal{B}^{\{s\}})$ for $s = 1, 2, \ldots, k$. Following a similar argument as that in section 4.2, the whole k-linear BGGK splits into k standard BGGKs started with different matricizations of $\mathcal{B}$. Schematically,

$$(\mathcal{B}, A_1, A_2, \ldots, A_k) \quad \xrightarrow{\text{BGGK}} \quad (\mathcal{B}_1, A_{1,11}, A_{2,11}, \ldots, A_{k,11}),$$

where $\mathcal{B}_1 \in \mathbb{R}^{\overline{m}_1 \times \overline{m}_2 \times \cdots \times \overline{m}_k}$ splits to

$$\begin{array}{llll}
[\mathcal{B}^{\{1\}}, A_1] & \xrightarrow{\text{BGGK}} & [B_{1,1}, A_{1,11}], \quad \text{where} & \mathcal{B}_1^{\{1\}} = B_{1,1}\widehat{M}_1^{\mathsf{T}}, \\
[\mathcal{B}^{\{2\}}, A_2] & \xrightarrow{\text{BGGK}} & [B_{2,1}, A_{2,11}], \quad \text{where} & \mathcal{B}_1^{\{2\}} = B_{2,1}\widehat{M}_2^{\mathsf{T}}, \\
 & \vdots & & \\
[\mathcal{B}^{\{k\}}, A_k] & \xrightarrow{\text{BGGK}} & [B_{k,1}, A_{k,11}], \quad \text{where} & \mathcal{B}_1^{\{k\}} = B_{k,1}\widehat{M}_k^{\mathsf{T}},
\end{array} \tag{4.13}$$

for some $\widehat{M}_s \in \mathbb{R}^{(\Delta/m_s) \times r_s}$, $\Delta = \prod_{\ell=1}^{k} \overline{m}_\ell$, $\widehat{M}_s^{\mathsf{T}} \widehat{M}_s = I_{r_s}$, for $s = 1, 2, \ldots, k$.

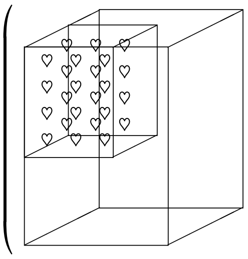
More precisely, the individual BGGK processes start with orthonormal bases of ranges of the particular matricizations of $\mathcal{B}$. Thus

$$P_{1,1:r_1} \equiv U'_1, \quad P_{2,1:r_2} \equiv U'_2, \quad \ldots, \quad P_{k,1:r_k} \equiv U'_k,$$

where P_s, $s = 1, 2, \ldots, k$, play roles of the orthogonal matrices from the CRT (2.9). Splitting the full k-linear process to the k standard BGGKs (4.13) results in right-hand sides matrices $B_{s,1}$ having full column rank, i.e., we naturally removed all the nonzero but linearly dependent fibers that may be present in the Tucker core (see the last paragraph of section 4.1), and zero fibers that may be present in the tensor $\mathcal{B}_1$ (similarly as zero columns and rows may appear in (4.11)).

To clarify the exposition, consider the example for $k = 3$, with the core problem right-hand side $\mathcal{B}_1 \in \mathbb{R}^{7 \times 5 \times 4}$ and with the Tucker core $\mathcal{B}_{\mathrm{TC}} \equiv \mathcal{B}_{1,\mathrm{TC}} \in \mathbb{R}^{4 \times 3 \times 2}$ (filled with hearts):

$(\mathcal{B}_1, A_{1,11}, A_{2,11}, A_{3,11}) =$



$$\left(\;\cdots\;, \left[\begin{array}{cccc}
\clubsuit & & & \\
\heartsuit & \clubsuit & & \\
\heartsuit & \heartsuit & & \\
\heartsuit & \heartsuit & \clubsuit & \\
\hline
\clubsuit & \heartsuit & \heartsuit & \clubsuit \\
 & \clubsuit & \heartsuit & \heartsuit \\
 & & \clubsuit & \heartsuit
\end{array}\right], \left[\begin{array}{cccc}
\clubsuit & & & \\
\heartsuit & \clubsuit & & \\
\heartsuit & \heartsuit & \clubsuit & \\
\hline
\clubsuit & \heartsuit & \heartsuit & \clubsuit \\
 & & \clubsuit & \heartsuit
\end{array}\right], \left[\begin{array}{ccc}
\clubsuit & & \\
\heartsuit & \clubsuit & \\
\hline
\clubsuit & \heartsuit & \clubsuit \\
 & \clubsuit & \heartsuit
\end{array}\right] \right).$$

Here
(4.14)

$$\mathcal{B}_1^{\{1\}} = \left[\begin{array}{cc|cc|c|c} \begin{matrix}\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit\end{matrix} & 0 & \begin{matrix}\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit\end{matrix} & 0 & \Huge 0 & \Huge 0 \\ 0 & 0 & 0 & 0 & & \end{array}\right] \in \mathbb{R}^{7\times(5\cdot 4)},$$

$$\mathcal{B}_1^{\{2\}} = \left[\begin{array}{cc|cc|c|c} \begin{matrix}\heartsuit&\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit&\heartsuit\end{matrix} & 0 & \begin{matrix}\heartsuit&\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit&\heartsuit\end{matrix} & 0 & \Huge 0 & \Huge 0 \\ 0 & 0 & 0 & 0 & & \end{array}\right] \in \mathbb{R}^{5\times(7\cdot 4)},$$

$$\mathcal{B}_1^{\{3\}} = \left[\begin{array}{cc|cc|cc|c|c} \begin{matrix}\heartsuit&\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit&\heartsuit\end{matrix} & 0 & \begin{matrix}\heartsuit&\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit&\heartsuit\end{matrix} & 0 & \begin{matrix}\heartsuit&\heartsuit&\heartsuit&\heartsuit\\ \heartsuit&\heartsuit&\heartsuit&\heartsuit\end{matrix} & 0 & \Huge 0 & \Huge 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & & \end{array}\right] \in \mathbb{R}^{4\times(7\cdot 5)},$$

are clearly not of full column ranks 4, 3, and 2, respectively. Recall $\widehat{M_s}$ matrices in (4.13), see also (4.6). The vertical lines in matricizations separate the individual frontal, transposed frontal, and transposed lateral slices of $\mathcal{B}_1$, respectively.

4.4. Note on QR-based variant of Tucker decomposition. For matrix right-hand side problems (ii), the decompositions of the $\mathrm{URV}^{\mathrm{T}}$ or $\mathrm{ULV}^{\mathrm{T}}$ forms (i.e., consecutive LQ and QR, or QR and LQ decompositions) can be used to preprocess B under a lower computational cost than with the use of SVD; see section 3.2. From the tensor point of view, we in fact obtain a QR decomposition in the first and second mode, respectively. Similarly, preprocessing of $\mathcal{B}$ can be improved.

Consider for simplicity a tensor of a small order, e.g., $\mathcal{B} = (b_{i_1,i_2,i_3}) \in \mathbb{R}^{8\times5\times4}$, $k = 3$. Recall how the matricization works on this example, i.e., how the individual entries are rearranged:

$$\mathcal{B}^{\{1\}} = \left[\begin{array}{ccc||ccc||ccc||ccc} b_{111} & \cdots & b_{151} & b_{112} & \cdots & b_{152} & b_{113} & \cdots & b_{153} & b_{114} & \cdots & b_{154} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ b_{811} & \cdots & b_{851} & b_{812} & \cdots & b_{852} & b_{813} & \cdots & b_{853} & b_{814} & \cdots & b_{854} \end{array}\right] \in \mathbb{R}^{8\times(5\cdot4)},$$

the individual blocks are $(1, 2)$-slices called for $k = 3$ frontal slices;

$$\mathcal{B}^{\{2\}} = \left[\begin{array}{ccc||ccc||ccc||ccc} b_{111} & \cdots & b_{811} & b_{112} & \cdots & b_{812} & b_{113} & \cdots & b_{813} & b_{114} & \cdots & b_{814} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ b_{151} & \cdots & b_{851} & b_{152} & \cdots & b_{852} & b_{153} & \cdots & b_{853} & b_{154} & \cdots & b_{854} \end{array}\right] \in \mathbb{R}^{5\times(8\cdot4)},$$

the individual blocks are $(2, 1)$-slices, i.e., here transposed frontal slices, and

$$\mathcal{B}^{\{3\}} = \left[\begin{array}{ccc||cc||c||cc||ccc} b_{111} & \cdots & b_{811} & b_{121} & \cdots & & \cdots & b_{841} & b_{151} & \cdots & b_{851} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \bullet\bullet\bullet & \ddots & \vdots & \vdots & \ddots & \vdots \\ b_{114} & \cdots & b_{811} & b_{124} & \cdots & & \cdots & b_{844} & b_{154} & \cdots & b_{854} \end{array}\right] \in \mathbb{R}^{4\times(8\cdot5)}$$

the individual blocks are $(3, 1)$-slices, i.e., here transposed lateral slices.

Further note that if $\mathcal{B}$ has zero cofibers in the ℓ mode (i.e., zero rows after unfolding into the ℓ-mode matricization), then application of a matrix in τ mode ($\tau \neq \ell$)

does not affect these zero cofibers. We illustrate this by employing QR decompositions on our example. First consider that, e.g.,

$$\operatorname{rank}(\mathcal{B}) = \Big(\operatorname{rank}(\mathcal{B}^{\{1\}})\,,\, \operatorname{rank}(\mathcal{B}^{\{2\}})\,,\, \operatorname{rank}(\mathcal{B}^{\{3\}})\Big) = (4,3,2).$$

Let $\mathcal{B}^{\{1\}} = Q_1 R_1$, where $Q_1^{-1} = Q_1^{\mathsf{T}} \in \mathbb{R}^{8\times 8}$, be the QR decomposition and, e.g.,

$$R_1 = \left[\begin{array}{ccccc||ccccc||c}
\clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \\
0 & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & & \cdots & & \heartsuit & \\
0 & 0 & \clubsuit & \heartsuit & \heartsuit & \heartsuit & & & & \heartsuit & \\
0 & 0 & 0 & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \bullet\bullet\bullet \\
\cline{1-10}
0 & & \cdots & & 0 & 0 & & \cdots & & 0 & \\
\vdots & & \ddots & & \vdots & \vdots & & \ddots & & \vdots & \\
0 & & \cdots & & 0 & 0 & & \cdots & & 0 &
\end{array}\right]. \tag{4.15}$$

By rearranging R_1 back into the original shape we get a tensor $\mathcal{R}_1$ satisfying $\mathcal{R}_1^{\{1\}} = R_1$ and $\mathcal{B} = Q_1 \times_1 \mathcal{R}_1$. Next consider the QR decomposition of

$$\mathcal{R}_1^{\{2\}} = \left[\begin{array}{cccc|ccc||cccc|ccc||c}
\clubsuit & 0 & 0 & 0 & 0 & \cdots & 0 & \heartsuit & \heartsuit & \heartsuit & \heartsuit & 0 & \cdots & 0 & \\
\heartsuit & \clubsuit & 0 & 0 & & & & \heartsuit & & & \heartsuit & & & & \\
\heartsuit & \heartsuit & \clubsuit & 0 & \vdots & \ddots & \vdots & \heartsuit & & \cdots & \heartsuit & \vdots & \ddots & \vdots & \bullet\bullet\bullet \\
\heartsuit & \heartsuit & \heartsuit & \clubsuit & & & & \heartsuit & & & \heartsuit & & & & \\
\heartsuit & \heartsuit & \heartsuit & \heartsuit & 0 & \cdots & 0 & \heartsuit & \heartsuit & \heartsuit & \heartsuit & 0 & \cdots & 0 &
\end{array}\right],$$

i.e., $\mathcal{R}_1^{\{2\}} = Q_2 R_2$, where $Q_2^{-1} = Q_2^{\mathsf{T}} \in \mathbb{R}^{5\times 5}$, and, e.g.,

$$R_2 = \left[\begin{array}{cccc|ccc||cccc|ccc||c}
\clubsuit & \heartsuit & \heartsuit & \heartsuit & 0 & \cdots & 0 & \heartsuit & \heartsuit & \heartsuit & \heartsuit & 0 & \cdots & 0 & \\
0 & \clubsuit & \heartsuit & \heartsuit & \vdots & \ddots & \vdots & \heartsuit & & \cdots & \heartsuit & \vdots & \ddots & \vdots & \\
0 & 0 & \clubsuit & \heartsuit & 0 & \cdots & 0 & \heartsuit & \heartsuit & \heartsuit & \heartsuit & 0 & \cdots & 0 & \bullet\bullet\bullet \\
\cline{1-14}
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 &
\end{array}\right], \tag{4.16}$$

and $\mathcal{R}_2$ satisfying $\mathcal{R}_2^{\{2\}} = R_2$ and $\mathcal{R}_1 = Q_2 \times_2 \mathcal{R}_2$, etc.

We see that for $\mathcal{B} \in \mathbb{R}^{n_1\times n_2\times\cdots\times n_k}$ with the rank$(\mathcal{B}) = (r_1, r_2, \ldots, r_k)$ any sequence of k QR decompositions in k distinct modes, e.g.,

$$\mathcal{B} \xrightarrow{\text{QR in mode } i_1} \mathcal{R}_{i_1} \xrightarrow{\text{QR in mode } i_2} \mathcal{R}_{i_2} \xrightarrow{\text{QR in mode } i_3} \quad \cdots \quad \xrightarrow{\text{QR in mode } i_k} \mathcal{R}_{i_k}$$

actually produces a QR-like Tucker decomposition

$$\mathcal{B} = Q_{i_1} \times_{i_1} (Q_{i_2} \times_{i_2} (\cdots \times_{i_{k-1}} (Q_{i_k} \times_{i_k} \mathcal{R}_{i_k}) \cdots)),$$

where $\mathcal{R}_k$ has a block diagonal structure

$$\mathcal{R}_k = \operatorname{diag}_k(\mathcal{R}_{k,\mathrm{TC}}, 0), \quad \text{and} \quad \mathcal{R}_{k,\mathrm{TC}} \in \mathbb{R}^{r_1\times r_2\times\cdots\times r_k}$$

is of full multilinear rank.

Since the R factor of a QR decomposition is in upper triangular row echelon forms, this structure is also visible on the core $\mathcal{R}_{k,\mathrm{TC}}$. However, it is clearly affected only by the last QR decompostion, as illustrated in Figures 4.1 and 4.2.

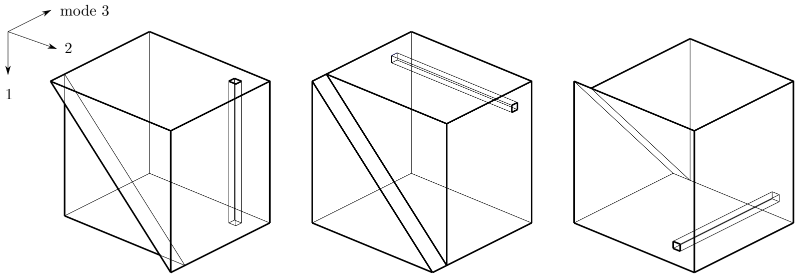


FIG. 4.1. *Structure of a Tucker core (here $k = 3$ and $r_1 = r_2 = r_k$) obtained by a sequence of QR decompositions. The last QR decomposition is in the mode $i_k = 1$ (left), 2 (middle), and 3 (right); one fiber in the respective mode is visualized. The upper triangular matrix R_{i_k} is considered to be in the same form as in* (4.15), (4.16), *i.e., with an invertible upper triangular block of the size r_{i_k}.*

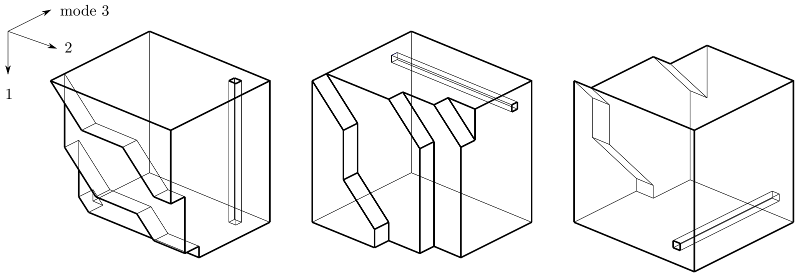


FIG. 4.2. *Similar illustration as in Figure* 4.1. *The upper triangular matrices R_{i_k} are considered to be in a more general row echelon form.*

5. Properties of subproblems obtained by BGGK.

It remains to show that the subproblems extracted by the methods described in sections 4.1, 4.2, and 4.3 represent the core problems. We prove this by showing that they satisfy the necessary and sufficient conditions (CP1)–(CP3); see sections 2.3 and 2.4, and, in particular, Theorem 2.3.

THEOREM 5.1. *Consider the problems*

$$A_{11} \times_1 \mathcal{X}_{11\ldots1} \approx \mathcal{B}_1,$$
$$A_{\mathrm{L},11} X_{11} A_{\mathrm{R},11}^{\mathsf{T}} \approx B_1,$$
$$(A_{1,11}, A_{2,11}, \ldots, A_{k,11} \,|\, \mathcal{X}_{11\ldots1}) \approx \mathcal{B}_1$$

obtained by the BGGK-based methods described in sections 4.1, 4.2, *and* 4.3, *respectively. These problems satisfy the defining conditions* (CP1)–(CP3). *Thus they represent core problems within the given data.*

Proof. Since the matrices of the reduced problems

$$A_{11}, \qquad A_{\mathrm{L},11},\ A_{\mathrm{R},11}, \qquad A_{1,11},\ A_{2,11},\ \ldots,\ A_{k,11},$$

are in a lower triangular column echelon form with no zero columns, they are of full column rank. Thus (CP1) is satisfied for all of them.

Now consider the tensor right-hand side problem (iii). Since we started the computation with the Tucker decomposition of $\mathcal{B}$, $\mathcal{B}_1$ is the Tucker core $\mathcal{B}_{\mathrm{TC}}$ of $\mathcal{B}$ with the first-mode fibers prolonged with zeros,

$$\mathcal{B}_1^{\{1\}} = \begin{bmatrix} \mathcal{B}_{\mathrm{TC}}^{\{1\}} \\ 0 \end{bmatrix},$$

and other dimensions unaffected. Thus $\mathcal{B}_1^{\{j\}}$, $j = 2, \ldots, k$ are of full row rank and consequently (CP2) holds.

To verify (CP3) for (iii) and (CP2)–(CP3) for (iv) and (v), we first point out that

$$A_{11}A_{11}^{\mathsf{T}}, \qquad A_{\mathrm{L},11}A_{\mathrm{L},11}^{\mathsf{T}},\ A_{\mathrm{R},11}A_{\mathrm{R},11}^{\mathsf{T}}, \qquad A_{1,11}A_{1,11}^{\mathsf{T}},\ A_{2,11}A_{2,11}^{\mathsf{T}},\ \ldots,\ A_{k,11}A_{k,11}^{\mathsf{T}},$$

are square, symmetric positive semidefinite matrices with a specific structure of nonzero entries called *wedge-shaped matrices*; see [16, Lemma 4.6] for the definition and details. Wedge-shaped matrices generalize the Jacobi tridiagonal matrices and have various interesting properties [12]. In particular,

- $A_{11}A_{11}^{\mathsf{T}}$ is r_1-wedge-shaped, where $r_1 = \mathrm{rank}_1(\mathcal{B})$;
- $A_{\mathrm{L},11}A_{\mathrm{L},11}^{\mathsf{T}}$ is r-wedge-shaped, where $r = \mathrm{rank}(B)$;
- $A_{\mathrm{R},11}A_{\mathrm{R},11}^{\mathsf{T}}$ is r-wedge-shaped, where $r = \mathrm{rank}(B)$; and
- $A_{s,11}A_{s,11}^{\mathsf{T}}$ is r_s-wedge-shaped, where $r_s = \mathrm{rank}_s(\mathcal{B})$, $s = 1, 2, \ldots, k$.

A multiplicity $\varrho(\lambda)$ of a real (and here nonegative) eigenvalue λ of a κ-wedge-shaped matrix $\Theta \in \mathbb{R}^{n \times n}$ is bounded by κ, $\varrho(\lambda) \le \kappa$; see [16] and [12]. Let $Z_\lambda \in \mathbb{R}^{n \times \varrho(\lambda)}$ be a matrix of $\varrho(\lambda)$ linearly independent eigenvectors of Θ corresponding to λ. Then the upper κ-by-$\varrho(\lambda)$ block of Z_λ, i.e.,

$$[I_\kappa, 0]^{\mathsf{T}} Z_\lambda \in \mathbb{R}^{\kappa \times \varrho(\lambda)},$$

is of full column rank; see [12, Corollary 5].

Now the eigenvalues of $A_{11}A_{11}^{\mathsf{T}}$ are squares of singular values of A_{11}, and the corresponding eigenvectors are left singular vectors of A_{11}. The condition (CP3) for (iii) requires that $U_i^{\mathsf{T}}\mathcal{B}_1^{\{1\}}$ are of full row rank for all i's. Since here $U_i \equiv Z_\lambda$ (originated in $A_{11}A_{11}^{\mathsf{T}}$) and $\mathcal{B}_1^{\{1\}} = \left[\begin{smallmatrix} W \\ 0 \end{smallmatrix}\right]$ with full row rank W equal to r_1, (CP3) holds.

Analogously, we can prove (CP2)–(CP3) for (iv). Using similar arguments to the above, here $U_{\mathrm{L},i} \equiv Z_\lambda$ (originated in $A_{\mathrm{L},11}A_{\mathrm{L},11}^{\mathsf{T}}$), $U_{\mathrm{R},j} \equiv Z_\lambda$ (originated in $A_{\mathrm{R},11}A_{\mathrm{R},11}^{\mathsf{T}}$), and $B_1 = \left[\begin{smallmatrix} \Sigma & 0 \\ 0 & 0 \end{smallmatrix}\right]$ and $\Sigma \in \mathbb{R}^{r \times r}$ are invertible. Consequently, $U_{\mathrm{L},i}^{\mathsf{T}}B_1$ and $U_{\mathrm{R},j}^{\mathsf{T}}B_1^{\mathsf{T}}$ are of full row rank for all i's and j's and (CP2)–(CP3) is satisfied.

Finally, in (v) we get $U_{s,i} \equiv Z_\lambda$ (originated in $A_sA_s^{\mathsf{T}}$). Furthermore, $\mathcal{B}_1^{\{s\}} = \left[\begin{smallmatrix} W \\ 0 \end{smallmatrix}\right]$ with the matrix W having full row rank equal to r_s, $s = 1, 2, \ldots, k$. Thus $U_{s,i_s}^{\mathsf{T}}\mathcal{B}_1^{\{s\}}$ are of full row rank for all i_s's and s's and (CP2)–(CP3) holds. □

The banded shape of the reduced problems determined by the described methods allows to formulate further properties of core problems. Note that the following theorem holds for core problems in general, i.e., it is not restricted to subproblems obtained by BGGK.

THEOREM 5.2 (property (CP6)–(CP7)). *Consider the core problems*

$$\begin{aligned} A_{11} \times_1 \mathcal{X}_{11\ldots1} &\approx \mathcal{B}_1, \\ A_{\mathrm{L},11} X_{11} A_{\mathrm{R},11}^{\mathsf{T}} &\approx B_1, \\ (A_{1,11}, A_{2,11}, \ldots, A_{k,11} \,|\, \mathcal{X}_{11\ldots1}) &\approx \mathcal{B}_1 \end{aligned}$$

obtained by the orthogonal transformations (2.7), (2.8), *and* (2.9), *respectively. Then the multiplicities of singular values of the matrices*

- A_{11} *are bounded by* $r_1 = \mathrm{rank}_1(\mathcal{B}_1)$*;*
- $A_{\mathrm{L},11}$ *and* $A_{\mathrm{R},11}$ *are bounded by* $r = \mathrm{rank}_1(B_1)$*;*
- $A_{s,11}$ *are bounded by* $r_s = \mathrm{rank}_s(\mathcal{B}_1)$*.*

The multiplicities of singular values of the extended matrices

- $[\mathcal{B}_1^{\{1\}}, A_{11}]$ *are bounded by* $r_1 = \mathrm{rank}_1(\mathcal{B}_1)$*;*
- $[B_1, A_{\mathrm{L},11}]$ *and* $[B_1^{\mathsf{T}}, A_{\mathrm{R},11}]$ *are bounded by* $r = \mathrm{rank}_1(B_1)$*;*
- $[\mathcal{B}_1^{\{s\}}, A_{s,11}]$ *are bounded by* $r_s = \mathrm{rank}_s(\mathcal{B}_1)$*.*

Proof. The proof again employs properties of wedge-shaped matrices. The first part follows directly from the fact that $A_{11}A_{11}^{\mathsf{T}}$ is an r_1-wedge-shaped matrix (and similarly for the other cases); see in particular [16, Lemma 4.6 and Corollary 4.3] or [12, Corollary 5].

The second assertion is a bit more complicated. Consider first the extended matrix $[\mathcal{B}_1^{\{1\}}, A_{11}]$, where $\mathrm{rank}(\mathcal{B}_1^{\{1\}}) = r$ (the other cases are analogous). The LQ decomposition of $\mathcal{B}_1^{\{1\}}$ gives $\mathcal{B}_1^{\{1\}} = [L, 0]Q^{\mathsf{T}}$, where L is lower triangular in the column echelon form with the full column rank r, and $Q^{\mathsf{T}} = Q^{-1}$. Then $[L, A_{11}]$ can be seen as an extended matrix of a core problem within some matrix right-hand side problem (ii). Thus it satisfies the properties (CP6)–(CP7) given in [16, Lemma 4.6] and [13, Theorem 2.2]; see also Appendix A. Since

$$[\mathcal{B}_1^{\{1\}}, A_{11}] = \left[\ [L, 0] \ \middle|\ A_{11}\ \right] \, \mathrm{diag}(Q^{\mathsf{T}}, I),$$

the assertion holds for all nonzero singular values. Finally, since the extended matrix is of full row rank (see the property (CP4)) it has no zero singular value. ∎

6. Conclusion.

In this paper we have introduced core problems within general multilinear approximation problems with a tensor right-hand side, and specified their defining properties. We described iterative methods providing core reduction of data for particular multilinear problems including the general one. This reduction can always be obtained by combining a specific preprocessing of the right-hand side data, followed by a series of independent block (or band) GK bidiagonalization processes applied on selected parts of the model and observation set. Properties of the reduced data ensure their minimality and uniqueness up to an orthogonal transformation. These results demonstrate that it is in principle possible to reduce maximally the given data by a procedure based on Krylov subspace projections. Computational aspects of the presented algorithms are behind the scope of this analytical paper and remain for future research.

Appendix A. The list of core problems properties.

In addition we list all the already known core problem properties for the problems (i)–(iv); for the details see [28], [15], [16], [17], and [18], respectively. We use the notation introduced in section 2.3. The properties that together form the necessary and sufficient condition for the minimality are asterisked.

- (i) The vector right-hand side core problem $A_{11}x_1 \approx b_1$; see [28]:
  - *(CP1) The matrix $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of full column rank equal to $\overline{n}$.
  - (CP2) The vector $b_1 \in \mathbb{R}^{\overline{m}}$ is nonzero.
  - *(CP3) The scalars $u_i^\mathsf{T} b_1 \in \mathbb{R}$ are nonzero (where u_i are the left singular vectors of A_{11}) for $i = 1,\ldots,\overline{m}$..
  - (CP4) The matrix $[b_1, A_{11}] \in \mathbb{R}^{\overline{m}\times(\overline{n}+1)}$ is of full row rank equal to $\overline{m}$.
  - (CP5) The scalars $e_1^\mathsf{T} v_\ell \in \mathbb{R}$ are nonzero (where e_1 is the first Euclidean vector and v_ℓ are the right singular vectors of $[b_1, A_{11}]$) for $\ell = 1,\ldots,\overline{n},\overline{n}+1$.
  - (CP6) Singular values of the matrix A_{11} are simple.
  - (CP7) Singular values of the matrix $[b_1, A_{11}]$ are simple.
  - (CP8) It always has a unique TLS solution.
- (ii) The matrix right-hand side core problem $A_{11}X_{11} \approx B_1$; see [15], [16]:
  - *(CP1) The matrix $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of full column rank equal to $\overline{n}$.
  - *(CP2) The matrix $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$ is of full column rank equal to $\overline{d}$.
  - *(CP3) Matrices $U_i^\mathsf{T} B_1 \in \mathbb{R}^{\overline{\mu}_i\times\overline{d}}$ are of *full row rank* $\overline{\mu}_i$, for $i = 1,\ldots,\overline{\xi},\overline{\xi}+1$.
  - (CP4) The matrix $[B_1, A_{11}] \in \mathbb{R}^{\overline{m}\times(\overline{n}+\overline{d})}$ is of full row rank equal to $\overline{m}$.
  - (CP5) The leading pricipal $\overline{d}\times\kappa_\ell$ blocks of V_ℓ are of full column rank κ_ℓ (where columns of V_ℓ span *either* the right singular vector subspace corresponding to the ℓth strictly largest nonzero singular value of $[B_1, A_{11}]$, *or* $\mathscr{N}([B_1, A_{11}])$).
  - (CP6) Multiplicities of singular values of A_{11} are bounded by $\overline{d}$.
  - (CP7) Multiplicities of singular values of $[B_1, A_{11}]$ are bouded nby $\overline{d}$.
  - (CP8) If it has a TLS solution, then it is unique.
- (iii) The tensor right-hand side core problem $A_{11} \times_1 \mathcal{X}_{11\ldots1} \approx \mathcal{B}_1$; see [17]:
  - *(CP1) The matrix $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of full column rank equal to $\overline{n}$.
  - *(CP2) The tensor $\mathcal{B}_1 \in \mathbb{R}^{\overline{m}\times\overline{d}_2\times\cdots\times\overline{d}_k}$ (where $\Delta \equiv \overline{m} \cdot \prod_{\ell=2}^{k} \overline{d}_\ell$) has the s-mode matricization $\mathcal{B}_1^{\{s\}} \in \mathbb{R}^{\overline{d}_s\times(\Delta/\overline{d}_s)}$ of full row rank equal to $\overline{d}_s$ (or, equivalently, all s-mode cofibers of $\mathcal{B}_1$ are linearly independent) for $s = 2,\ldots,k$.
  - *(CP3) Matrices $U_i^\mathsf{T} \mathcal{B}_1^{\{1\}} \in \mathbb{R}^{\overline{\mu}_i\times(\Delta/\overline{m})}$ are of full row rank $\overline{\mu}_i$ for $i = 1,\ldots,\overline{\xi},\overline{\xi}$ $+1$.
  - (CP4) The matrix $[\mathcal{B}_1^{\{1\}}, A_{11}] \in \mathbb{R}^{\overline{m}\times(\overline{n}+\Delta/\overline{m})}$ is of full row rank equal to $\overline{m}$.
- (iv) The bilinear core problem $A_{\mathrm{L},11}X_{11}A_{\mathrm{R},11} \approx B_1$; see [18]:
  - *(CP1) The matrix $A_{\mathrm{L},11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of full column rank equal to $\overline{n}$.
    The matrix $A_{\mathrm{R},11} \in \mathbb{R}^{\overline{d}\times\overline{c}}$ is of full column rank equal to $\overline{c}$.
  - *(CP2) Matrices $B_1 U_{\mathrm{R},j} \in \mathbb{R}^{\overline{m}\times\overline{\gamma}_j}$ are of full column rank $\overline{\gamma}_j$, $j = 1,2,\ldots,\overline{\zeta},\overline{\zeta}+1$.
  - *(CP3) Matrices $U_{\mathrm{L},i}^\mathsf{T} B_1 \in \mathbb{R}^{\overline{\mu}_i\times\overline{d}}$ are of full row rank $\overline{\mu}_i$, $i = 1,2,\ldots,\overline{\xi},\overline{\xi}+1$.
  - (CP4) The matrix $[B_1, A_{\mathrm{L},11}] \in \mathbb{R}^{\overline{m}\times(\overline{n}+\overline{d})}$ is of full row rank equal to $\overline{m}$.
    The matrix $[B_1^\mathsf{T}, A_{\mathrm{R},11}] \in \mathbb{R}^{\overline{d}\times(\overline{c}+\overline{m})}$ is of full row rank equal $\overline{d}$.

Acknowledgment. The authors wish to thank the anonymous referees for their useful comments that helped to improve this paper.

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CONCLUSIONS

In this thesis we have studied linear approximation problems of different forms, the core problems within them, and partially also their solvability in the TLS sense. The main motivation for us is that the core problem with matrix right-hand side may not have a TLS solution.

In Part II we have built up very general and robust algebraic framework enabling to handle and study internal structure of core problems with matrix right-hand sides. That led us to some rather simple or partial, but anyway interesting results — for example the interpretation of the core problem reduction as the orthogonal projection from the set of all linear approximation problems onto the set of core problems, or the commutation of the core problem reduction with the problem composition (see Section 5.2.3). It also allowed us to formulate and partially also answer the question on irreducible representation of linear approximation problem (in terms of composition) (see Section 5.3.6). As a by-product we have described in details how to extract the degenerated component (that can be seen as the part of the problem that only increases residuum) from the core problem (see Section 5.3.3). Our journey into the internal structure of core problems is complemented by already published work [10] (see page 83) that analyzes the evolution of TLS solvability of core problems while composing.

There are, however, two main open questions related to the results presented in Part II. First, it is still not clear how the irreducible representation of the proper core problem looks like (our partial answer to the irreducible representation is related to its easier part); it is also not clear how the general irreducible core problem (possibly with given number of right-hand sides $\overline{d} \geq 2$) looks like. The second open question relates to our work [10], where we analyze only a few selected combinations; further combinations or more sophisticated analysis is missing.

In Part III we did in particular the analysis of the existence and uniqueness of the core problem within three different (but related) linear approximation problems: problems with tensor right-hand side, bilinear problems with matrix right-hand side, and multilinear problems with tensor right-hand side. All of them can be seen as generalizations of the matrix right-hand side problem (and generalizations or specializations of themselves). All three core problem reductions are also already published in [8] (see page 141), [9] (see page 167), and [11] (see page 187), respectively. The core problem revealing orthogonal transformation is in all three cases essentially done via the SVD of the mapping (which is either a single matrix, or Kronecker product of matrices). In the last paper we also propose the Krylov subspace approach based on the band generalization of the Golub–Kahan iterative bidiagonalization (which in fact can be due to the specialization directly applied on all three cases); this is, however, not in the main interest of this thesis.

Note that there are interesting and important open questions related to Part III, too. In particular, the TLS solvability theory for bilinear and multilinear problem is not fully resolved yet, up to our knowledge (see Remarks 6 and 8). Both approaches can be also combined and one could ask about irreducible representations of these generalizations (note that our algebraic framework is already fully prepared for the bilinear problems). These open questions will be addressed in the future work.

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A BRIEF INFORMATION ABOUT SCIENTIFIC ACHIEVEMENTS OF THE APPLICANT

A.1 LIST OF ALL PAPERS IN WOS-INDEXED JOURNALS

All co-authors of each of the items listed below participate on the results in equal share.

1. I. Hnětynková, M. Plešinger, and J. Žáková, *Filter factors of truncated TLS regularization with multiple observations*, Applications of Mathematics 62 (2) (2017), pp. 105–120.

   `https://link.springer.com/article/10.21136/am.2017.0228-16`

   Not directly related to this thesis.

   One relevant citation:

   - P. Xie, H. Xiang, Y. Wei, *Randomized algorithms for total least squares problems*, NLAA (WoS) (2018).
     `https://doi.org/10.1002/nla.2219`

2. I. Hnětynková, M. Plešinger, and J. Žáková, *TLS formulation and core reduction for problems with structured right-hand sides*, Linear Algebra and its Applications 555 (2018), pp. 241–265.

   `https://www.sciencedirect.com/science/article/pii/S0024379518303008`

   See also page 141, or reference [8].

   One relevant citation:

   - L. Zhang, Y. Wei, *Randomized core reduction for discrete ill-posed problem*, JCAM (WoS) (2020).
     `https://doi.org/10.1016/j.cam.2020.112797`

3. I. Hnětynková, M. Plešinger, and J. Žáková, *Solvability classes for core problems in matrix total least squares minimization*, Applications of Mathematics 64 (2) (2019), pp. 103–128.

   https://link.springer.com/article/10.21136/am.2019.0252-18

   See also page 83, or reference [10].

   Two relevant citations:

   - V. A. Gorelik, T. V. Zolotova, *The total method of Chebyshev interpolation in the problem of constructing a linear regression* (in Russian), Chebyshevskii Sbornik (not in WoS) (2022).
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   - H. Zhou, *An iterative algorithm to the least squares problem of* $AX = B$ *over linear subspace* (in Chinese), Mathematica Numerica Sinica (not in WoS) (2023).
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4. I. Hnětynková, M. Plešinger, and J. Žáková, *On TLS formulation and core reduction for data fitting with generalized models*, Linear Algebra and its Applications 577 (2019), pp. 1–20.

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   See also page 167, or reference [9].

   One relevant citation:

   - V. A. Gorelik, T. V. Zolotova, *The total method of Chebyshev interpolation in the problem of constructing a linear regression* (in Russian), Chebyshevskii Sbornik (not in WoS) (2022).
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5. I. Hnětynková, M. Plešinger, and J. Žáková, *Krylov subspace approach to core problems within multilinear approximation problems: A unifying framework*, SIAM Journal on Matrix Analysis and Applications 44 (1) (2023), pp. 53–79.

   https://epubs.siam.org/doi/abs/10.1137/21M1462155

   See also page 187, or reference [11].

A.2 LIST OF OTHER PUBLICATIONS (OTHER PEER-REVIEWED JOURNALS & CONFERENCE PROCEEDINGS

All co-authors of each of the items listed below participate on the results in equal share.

1. I. Hnětynková, M. Plešinger, and J. Žáková, *Modification of TLS algorithm for solving $\mathscr{F}_2$ linear data fitting problems*, Proceedings in Applied Mathematics and Mechanics 17 (1) (2017), pp. 749–750.

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   See also page 35, or reference [12].

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   Special issue: 89th GAMM Annual Meeting, München 2018.

   Conference presentation given by JŽ.

   `https://doi.org/10.1002/pamm.201800196`

3. I. Hnětynková, M. Plešinger, and J. Žáková, *Extracting relevant data from linear data fitting problems via generalized Krylov subspace methods*.

   Proceedings of XXI Householder Symposium on Numerical Linear Algebra, Selva di Fasano 2020/2022, pp. 219–221.

   Conference presentation given by IH.

   `https://users.ba.cnr.it/iac/irmanm21/HHXXI/book_of_abstracts_HHXXI0.pdf#page=219`

4. I. Hnětynková, M. Plešinger, and J. Žáková, *Recent development of the core problem theory in the context of the total least squares minimization*.

   Proceedings of XXI Householder Symposium on Numerical Linear Algebra, Selva di Fasano 2020/2022, pp. 321–323.

   Conference presentation given by MP.

   `https://users.ba.cnr.it/iac/irmanm21/HHXXI/book_of_abstracts_HHXXI0.pdf#page=321`

A.3 LIST OF CONFERENCE PRESENTATIONS (TALKS & POSTERS)

1. *Total least squares problem and its tensor generalizations* (talk), PANM 18 — Programy a algoritmy numerické matematiky 18, Janov nad Nisou, 2016.
2. *Selected tensor generalizations of total least squares* (talk), 89th GAMM Annual Meeting, München, 2018.
3. *The total least squares and the core problem in tensor settings* (talk), GAMM ANLA — GAMM Workshop Applied and Numerical Linear Algebra, Chemnitz, 2019.
4. *Selected recent outcomes in the theory of core problems in tensor settings* (talk), PANM 20 — Programy a algoritmy numerické matematiky 20, Hejnice, 2020.
5. *Recent development of the core problem theory in the context of the total least squares minimization* (poster), PANM 22 — Programy a algoritmy numerické matematiky 22, Jablonec nad Nisou, 2022.

A.4 LIST OF PROJECTS

All projects in this list are one-year internal TUL, resp. FP TUL grants for supporting master or PhD students. The team usually consists of the student (as the team-leader) and her advisor; two exceptions are explicitly mentioned.

1. TUL-FP-SGS/2016/21161: *Total least squares problem and its tensor generalizations* (with Martin Plešinger as the team-leader).
2. TUL-FP-SGS/2018/21254: *Tensor methods and their analysis in numerical linear algebra*.
3. TUL-FP-SGS/2019/21319: *Numerical methods in matrix and tensor computations*.
4. SGS-2020-4022: *Krylov subspace methods in core problem theory*.
5. SGS-2021-4039: *Krylov methods in tensor problems*.
6. SGS-2022-4025: *Mathematical modeling and data analysis* (together with Čeněk Jirsák as the third team member).