Czech University of Life Sciences Prague
Faculty of Environmental Sciences
Department of Water Resources and Environmental Modeling

Thesis extended summary

Application of optimization methods in hydrological modelling

Ing. Michala Jakubcová

Supervisor: doc. Ing. Petr Máca, Ph.D.

Prague 2015

Doktorská disertační práce “Application of optimization methods in hydrological modeling” byla vypracována v rámci doktorského studia na Katedře vodního hospodářství a environmentálního modelování Fakulty životního prostředí České zemědělské univerzity v Praze.

Uchazečka: Ing. Michala Jakubcová
Obor: Environmentální modelování
Školitel: doc. Ing. Petr Máca, Ph.D.

Oponenti:
doc. Ing. Martin Hanel, Ph.D. - Fakulta životního prostředí ČZU v Praze
Ing. Ladislav Kašpárek, CSc. - Výzkumný ústav vodohospodářský TGM, v.v.i.
Ing. Tomáš Metelka, Ph.D. - DHI a.s.

Autoreferát byl rozeslán dne: 11. 11. 2015

Obhajoba disertační práce se koná dne 3. prosince 2015 v 10:00 v místnosti L264 Fakulty životního prostředí České zemědělské univerzity v Praze, Kamýcká 129, Praha 6 - Suchdol.

S disertační prací je možné se seznámit na Oddělení pro vědu a výzkum FŽP ČZU v Praze, Kamýcká 129, Praha 6 - Suchdol.

Table of Contents

Chapter 1

Introduction

Optimization is a process in which the best variant from many possibilities is chosen. It is very important for increasing effectiveness, or decreasing demands of the computational system.

The optimization process could be very complicated. The main challenges, which can make the process of finding the optimal value of a given objective function more difficult, are [19]:

- premature convergence to a local optimum,
- noisy function with no useful information about the gradient of the function,
- unexpected shape of the function with sudden change of the course,
- function with long slight declining or increasing section, which resembles a constant function.

Therefore, it is necessary to wisely choose a suitable optimization method, and devote some time to its modification according to the given problem.

This doctoral thesis is focused on optimization used in hydrological modelling. The applied and analysed technique chosen within this thesis is method called particle swarm optimization (PSO). It is inspired by behaviour of social organisms in the nature. The main advantages are low number of parameters, which need to be adjusted, and no requirement of knowledge about gradient of the optimized function [9].

1.1 Main goals

Particle swarm optimization was analysed within this doctoral thesis due to its advantages. The PSO was successfully used in many real life case studies, and its applicability and efficiency were proved. It is relatively recent optimization technique, and thus, new modifications can be made to improve its optimization ability.

Main goals of the doctoral thesis are following:

- provide a literature review about the particle swarm optimization method with emphasis to its utilization in hydrological modelling,
- create algorithms of different modified versions of PSO with the implementation in C++ programming language,
- propose new algorithm of PSO, and implement it in C++ programming language,
- test the existing PSO modifications with the new proposed variant on chosen benchmark objective functions,
- applied the best PSO algorithms on case studies regarding rainfall-runoff simulations and training artificial neural networks.

This doctoral thesis will extend the range of global optimization techniques. The results will contribute to utilization of PSO method in real-life optimization problems. New algorithms will have high application potential not only in the field of hydrological modelling. Completed algorithms become basis for other research projects, and they will be available for later use.

Chapter 2

Particle swarm optimization in hydrological modelling

2.1 Introduction to optimization

Optimization is a process which serves to find the optimal values of mathematical function. In many cases, the problem is searching for extremes of the function. The optimization problem is defined by function f, and by n-dimensional search space $\mathbb{R}^n$. The function f is called an *objective*, *error*, or *fitness function*. The problem can be defined as

$$f : \mathbb{R}^n \to \mathbb{R}. \tag{2.1}$$

If the optimization problem is a minimization of the objective function, the algorithm searches for the minimal value $\mathbf{X_{min}} \in \mathbb{R}^n$, for which [18]

$$\forall \mathbf{X} \in \mathbb{R}^n : f(\mathbf{X_{min}}) \leq f(\mathbf{X}). \tag{2.2}$$

The main aim of optimization is to find the best set of parameters of the objective function in an acceptable amount of time. This process is very important in many professions.

2.1.1 Optimization methods

The solution of optimization problem can be found through many optimization methods. Probabilistic methods of meta-heuristic technique are based on populations. In this approach, many individuals, which represent possible solutions of the objective function, are stored in the memory. Evolutionary computation

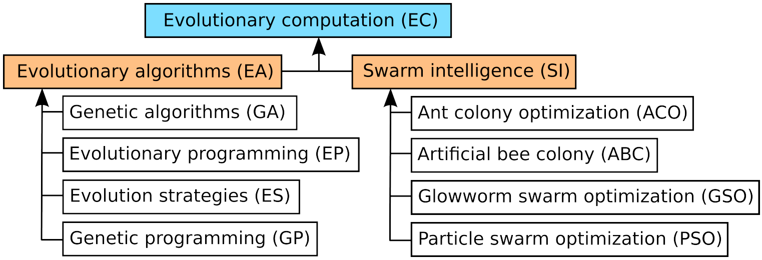

Figure 2.1: Simplified system of evolutionary computation technique (adapted from [18])

(EC) is one of the largely explored probabilistic method. The simplified system of this technique is depicted on Figure 2.1.

2.1.2 Swarm intelligence

Particle swarm optimization (PSO) is one of the optimization method along with ant colony optimization [2], glowworm swarm optimization [10], or artificial bee colony algorithm [8], which is part of the swarm intelligence (SI) technique.

In the SI, each individual of a social community (e.g. ant, termite, bee, fish, bird, etc.) is usual, but as a unit they are able to accomplish a complicated task due to mutual cooperation [3]. The behaviour of organisms follows three simple rules [16]:

- *separation* - to avoid an overcrowding and collision (Fig. 2.2a),
- *cohesion* - to stay close to the neighbours (Fig. 2.2b),
- *alignment* - to match the direction and magnitude of velocity vector with the neighbours (Fig. 2.2c).

2.2 Original equations

Particle swarm optimization is inspired by successive and unpredictable fly of birds [9]. The method has only a few parameters to adjust, and it is relatively easy to implement and use. The main advantage is also the fact, that PSO does

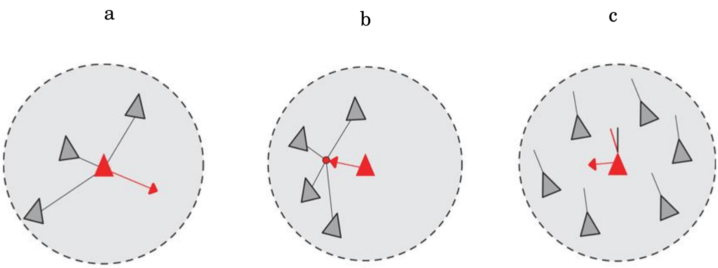

Figure 2.2: Rules of behaviour in SI, a) separation, b) cohesion, c) alignment [11]

not need gradient information of the objective function during the iterative search [7, 12, 13].

PSO contains a population of particles $i = 1, ..., S$, where S is total number of individuals. Particles represent a potential solution of the optimization problem, and every new generation of individuals is closer to the searched optimum. The problem space has dimension $d = 1, ..., Dim$, where Dim is total number of parameters.

Each particle i has its own position $\mathbf{X_i} = (\mathbf{x_1^i}, \mathbf{x_2^i}, ..., \mathbf{x_{Dim}^i})$ in the space, and velocity $\mathbf{V_i} = (\mathbf{v_1^i}, \mathbf{v_2^i}, ..., \mathbf{v_{Dim}^i})$, which are stored in the memory. Each particle i also maintains its previous best position $\mathbf{P_i} = (\mathbf{p_1^i}, \mathbf{p_2^i}, ..., \mathbf{p_{Dim}^i})$, and the best position among all particles $\mathbf{G} = (\mathbf{g_1}, \mathbf{g_2}, ..., \mathbf{g_{Dim}})$ [4, 6, 9].

The original PSO algorithm consists of two main equations. One equation is for computing particle's velocity

$$\mathbf{v_d^i}(t+1) = \mathbf{v_d^i}(t) + c_1 \cdot \mathbf{r_{1d}}(t) \cdot (\mathbf{p_d^i}(t) - \mathbf{x_d^i}(t)) + c_2 \cdot \mathbf{r_{2d}}(t) \cdot (\mathbf{g_d}(t) - \mathbf{x_d^i}(t)), \quad (2.3)$$

and the second equation calculates particle's position

$$\mathbf{x_d^i}(t+1) = \mathbf{x_d^i}(t) + \mathbf{v_d^i}(t+1), \quad (2.4)$$

where t is time step, $\mathbf{r_{1d}}$ and $\mathbf{r_{2d}}$ are members of vectors $\mathbf{R1}$ and $\mathbf{R2}$ of random numbers uniformly distributed in the range of $[0, 1]$, respectively, c_1 and c_2 are acceleration constants predefined by the user.

2.3 Modifications of PSO

In the optimization process, the premature convergence could appear, where the model could converge to the local optimum instead of the global one. Many researches were devoted avoiding this phenomenon [1, 14, 15].

The original PSO equation for calculating particle's velocity was modified to improve the optimization performance of the algorithm. The velocity from the previous time step is updated by a given parameter. The parameter is inertia weight, or constriction factor.

Other possibility for increasing the optimization ability is to use distributed version of the algorithm. In this approach, the population is divided into several complexes, where the PSO algorithm runs at each complex individually.

2.4 Objective functions

During optimization, the main aim is to find an optimal value of an objective function f. For testing and comparison purposes, the benchmark problems are solved. Optimization based on hydrological indexes is commonly used in practical experiments within the field of hydrological modelling.

2.4.1 Benchmark problems

Benchmark problems serve for comparing different optimization techniques, or for testing new proposed optimization method. Benchmark functions are precisely defined, the user knows their formula, range of the search space, and the position of the optimal value. Results of finding the optimal value are comparable across different research for all scientists.

2.4.2 Hydrological indexes

Optimization methods in hydrological modelling are used for calibration of models, estimation of rainfall-runoff relationships, meteorological forecasts, or runoff predictions. Hydrological index serves as an objective function, and it can also determines the quality of hydrological model.

Chapter 3

A comparison of selected modifications of the particle swarm optimization algorithm

In this chapter, 27 modifications of the original particle swarm optimization (PSO) algorithm are compared. The analysis evaluated nine basic PSO types, which differ according to the swarm evolution as controlled by various inertia weights and constriction factor. Each of the basic PSO modifications was analysed using three different distributed strategies. In the first strategy, the entire swarm population is considered as one unit (OC-PSO). The second strategy periodically partitions the population into equally large complexes according to the particle's functional value (SCE-PSO). The final strategy periodically splits the swarm population into complexes using random permutation (SCERand-PSO). All variants were tested using 11 benchmark functions.

This chapter is based on the publication: JAKUBCOVÁ M., MÁCA P., AND PECH P., 2014: A comparison of selected modifications of the particle swarm optimization algorithm. *Journal of Applied Mathematics*, vol. 2014, Article ID 293087, 10 pp, doi: 10.1155/2014/293087.

Table 3.1: Summary of PSO modifications

Label	Equation
AdaptW	$w = (w_{max} - w_{min}) \cdot P_s + w_{min}$
ChaoticRandW	$w(iter) = 0.5 \cdot rand() + 0.5 \cdot z$
ChaoticW	$w(iter) = (w_{max} - w_{min}) \cdot \frac{iter_{max} - iter}{iter_{max}} + w_{min} \cdot z$
ConstantW	$w = c$
ConstrFactor	$K = \frac{2}{\lvert 2 - \varphi - \sqrt{\varphi^2 - 4 \cdot \varphi} \rvert}$
LinTimeVaryingW	$w(iter) = \frac{iter_{max} - iter}{iter_{max}} \cdot (w_{max} - w_{min}) + w_{min}$
NonlinTimeConstW	$w(iter) = w_{ini} \cdot u^{iter}$
NonlinTimeW	$w(iter) = \left(\frac{2}{iter} \right)^{0.3}$
RandomW	$w = 0.5 + \frac{rand()}{2}$

3.1 Methodology

In the present study, nine variants of PSO algorithm were used and tested (Tab. 3.1), including eight modifications using inertia weight parameter w, and one modification with constriction factor K.

All nine modifications are used with three strategies of swarm distribution. Changes in behaviour of the population for each modification and strategy were observed. The first distributed strategy considered the whole population as one unit called OC-PSO. In the next swarm distributions, the population was divided into several complexes according to the particle's functional value (SCE-PSO), or through random permutation (SCERand-PSO).

For comparison purposes, 11 benchmark functions prepared for the special session on real-parameter optimization of CEC 2005 [17] were used. All functions have shifted global optima, some of them is rotated, or with noise. The aim is to find the minimum of all functions.

3.2 Results

The non-parametric Wilcoxon test was used for statistical comparison. Inputs to those calculations were the best fitness values achieved for all modifications. The null hypothesis H_0 of the Wilcoxon test is that differences between algorithms have a median of zero.

The strategy SCE-PSO produced the best solution in seven functions. Strategy SCERand-PSO produced the best solution in two functions (f_9,f_{10}), and in one function (f_5), the best solution was from strategy OC-PSO. For function f_1, there was no significant difference between strategy SCE-PSO and SCERand-PSO.

Upon closer examination, “AdaptW” and “NonlinTimeConstW” are the best modifications for unimodal functions (f_1 - f_5). The poorest variants are “ConstantW” and “ConstrFactor”. The best PSO modification for multimodal functions (f_6 - f_{11}) is “AdaptW”, and the poorest is “ConstantW”.

For rotated functions (f_3, f_7, f_8, f_{10}, f_{11}), the best modification of the PSO algorithm appears to be “AdaptW”, and the poorest is “CostantW”. For functions where there is no transformation matrix to rotate them, is the best variant “AdaptW”, and the poorest are “ConstantW” and “ConstrFactor”.

It is clear that the best modification of the particle swarm optimization algorithm for the selected benchmark functions is “AdaptW”, i.e. adaptive inertia weight. The variant called “NonlinTimeConstW” also produced good results. On the other hand, the poorest modifications appear to be “ConstantW” and “ConstrFactor”.

3.3 Conclusions

The main aim of this work was to find the global minima of 11 benchmark functions prepared for the special session on real-parameter optimization of CEC 2005. In total, 27 variants of particle swarm optimization algorithm were compared. Eight modifications were performed using the parameter inertia weight, and one modification using constriction factor. All modifications were tested with three strategies of swarm distribution, which were in terms of population. The population was either considered as a single unit, or it was divided into several complexes.

The best modification of the PSO algorithm is the variant called “AdaptW”. The best choice for selected benchmark functions is to use the parameter of inertia weight, where the w value is adapted based on a feedback parameter.

The best strategy for swarm distribution is SCE-PSO. Shuffled complex evolution particle swarm optimization with allocation of particles into complexes according to their functional values is better than OC-PSO and SCERand-PSO. The original particle swarm optimization has slow convergence to the global optimum, and the shuffling mechanism improves the optimization.

Chapter 4

Parameter estimation in rainfall-runoff modelling using distributed versions of particle swarm optimization algorithm

This chapter provides the analysis of selected versions of the particle swarm optimization (PSO) algorithm. The tested versions of the PSO were combined with the shuffling mechanism, which splits the model population into complexes, and performs distributed PSO optimization. One of them is a new proposed PSO modification - APartW, which enhances the global exploration and local exploitation in the parametric space during the optimization process through the new updating mechanism applied on the PSO inertia weight. The performances of four selected PSO methods were tested on 11 benchmark optimization problems. The distributed PSO versions were developed for finding the solution of inverse problems related to the estimation of parameters of hydrological model Bilan.

This chapter is based on the publication: JAKUBCOVÁ M., MÁCA P., AND PECH P., 2015: Parameter estimation in rainfall-runoff modelling using distributed versions of particle swarm optimization algorithm. *Mathematical Problems in Engineering*, vol. 2015, Article ID 968067, 13 pp, doi: 10.1155/2015/968067.

4.1 Methodology

In total, 4 versions of the PSO algorithm were analysed. They differ according to applied particle's velocity adaptation. The modifications are called ConstrFactor, LinTimeVarW, AdaptW, and APartW. The APartW is the new proposed variant, which combines the global exploration and local exploitation in the space. All four PSO variants were extended into a distributed version using SCE-PSO technique.

The distributed versions of PSO were tested on two sets of single-objective optimization problems. The first set is represented by 11 benchmark problems, which were specially prepared for CEC 2005 single-objective optimization session [17]. The second set consists of 120 optimization problems. On 30 datasets of MOPEX catchments, 4 benchmark questions were evaluated, which are standard objective functions used for solving inverse problem related to calibrations of hydrological models.

4.2 Results

The results of the statistical analysis of the benchmark problems show that the APartW modification gives significantly better results for three benchmark functions (f_4, f_7 and f_{11}). In functions f_3, f_5 and f_9, there is no significant difference between APartW and AdaptW. Beyond that, in functions f_1 and f_2, both APartW and AdaptW found the global minimum. For multi-modal functions f_6, f_8 and f_{10}, the AdaptW variant gives significantly better results.

Table 4.1 displays results from the contrast test of the unadjusted medians for Bilan calibration according to [5]. After pairwise comparison of all PSO modifications, the ranks of each method were determined. The best method seems to be the AdaptW, which achieved the best results two times and the second rank also two times. On the other hand, the worst is the ConstrFactor version, which was always worse than the others. Additionally, differences in medians between LinTimeVarW, AdaptW and APartW are very small, which indicates similar performances.

In addition to the contrast test, the Wilcoxon pair test of medians was conducted. The ranks are displayed in the last column in Table 4.1. The obtained

Table 4.1: The contrast test of the unadjusted medians with ranking. The $Rank$ is ranking based of contrast test, $W.Rank$ is ranking based of Wilcoxon pair test

MSE	ConstrFactor	LinTimeVarW	AdaptW	APartW	Rank	W.Rank
ConstrFactor	-	372.66	373.23	373.22	4	4
LinTimeVarW	-372.66	-	0.57	0.55	3	3
AdaptW	-373.23	-0.57	-	-0.01	1	2
APartW	-373.22	-0.55	0.01	-	2	1
MAE	ConstrFactor	LinTimeVarW	AdaptW	APartW	Rank	W.Rank
ConstrFactor	-	374.78	374.82	374.82	4	4
LinTimeVarW	-374.78	-	0.04	0.04	3	3
AdaptW	-374.82	-0.04	-	0.00	2	2
APartW	-374.82	-0.04	-0.00	-	1	1
MAPE	ConstrFactor	LinTimeVarW	AdaptW	APartW	Rank	W.Rank
ConstrFactor	-	374.96	375.02	375.02	4	4
LinTimeVarW	-374.96	-	0.06	0.05	3	3
AdaptW	-375.02	-0.06	-	-0.00	1	1-2
APartW	-375.02	-0.05	0.00	-	2	1-2
NS	ConstrFactor	LinTimeVarW	AdaptW	APartW	Rank	W.Rank
ConstrFactor	-	375.01	374.91	374.91	4	4
LinTimeVarW	-375.01	-	-0.10	-0.10	1	1
AdaptW	-374.91	0.10	-	-0.00	2	2
APartW	-374.91	0.10	0.00	-	3	3

results confirm the results from the contrast test. The differences in the ranks are in the simulations based on mean squared error (MSE) and mean absolute percentage error ($MAPE$) objective functions, where APartW variant is better than the AdaptW, or as good as AdaptW, respectively. In terms of Wilcoxon test, the APartW is the best modification and ConstrFactor is again the worst.

On Figure 4.1 is displayed the time series of observed and modelled runoff using APartW method. It gives an example of ensemble simulations with the Bilan model, where the results from the total 25 model runs are coloured in grey. It is evident that the envelope curve of the ensemble simulations would cover most of the observed data points. On the figure, also the streamflow calculated by the best model is plotted (red line), i.e. the simulation with the highest value of Nash-Sutcliffe efficiency (NS).

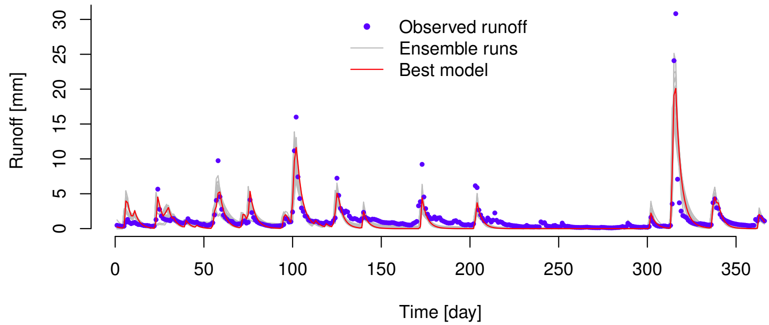

Figure 4.1: Observed streamflow and corresponding simulations from Bilan model using APartW optimization. The optimized objective function was NS. Catchment 01531000, year 1976

4.3 Conclusions

The main aim of this chapter was to test 4 selected PSO distributed versions on single-objective benchmark optimization problems, and to apply them on calibration of hydrological model Bilan. For all 4 PSO versions, 3 275 optimization problems were analysed, in which 275 minimizations for benchmark problems (i.e. 11 benchmark function × 25 program runs) and 3 000 inverse hydrological problems (i.e. 4 objective functions × 30 catchments × 25 program runs) were solved.

The new proposed variant APartW was compared with other existing PSO modifications - ConstrFactor, LinTimeVarW and AdaptW on 11 benchmark functions prepared for the special session on real-parameter optimization of CEC 2005. The APartW version is comparable with the AdaptW and LinTimeVarW variants, whereas the ConstrFactor had the worst performance.

All four PSO modifications were implemented into the Bilan rainfall-runoff model for solving inverse hydrological problems. Based on the contrast test of the unadjusted medians and Wilcoxon test, it was found out that the APartW and AdaptW variants provided the best results. The ConstrFactor performed the worst.

The results highlighted that distributed versions of PSO are promising in single-objective optimization problems. It was confirmed that adaptive variants of the inertia weight are better then linearly decreasing weight. It was also found out that the PSO modifications with parameters of inertia weight give significantly better results than the variant with constriction factor.

Chapter 5

Combination of hybrid artificial neural networks with particle swarm optimization algorithm for SPEI forecasting

The recent climatic water balance indicator, the Standardized precipitation evapotranspiration index (SPEI), was forecasted within this chapter. New tool for the SPEI simulations was proposed, which is a combination of hybrid artificial neural networks (ANN) with particle swarm optimization (PSO). The PSO algorithm was used for training the model weights to achieve higher accuracy in shorter computational time. In this research, the influence of chosen PSO modifications, number of inputs into the ANN, number of neurons in the hidden layer, and influence of the type of optimized objective function on modelled SPEI drought index were evaluated. The case study was conducted on selected set of 8 US catchments with the data of meteorological observations obtained from MOPEX database.

This chapter is based on the manuscript: JAKUBCOVÁ M., MÁCA P., AND PECH P., 2015: Combination of hybrid artificial neural networks with particle swarm optimization algorithm for SPEI forecasting. *Applied Soft Computing*.

5.1 Methodology

The combination of hybrid artificial neural network models with particle swarm optimization technique was applied for forecasting the SPEI drought index. The models differ in four variables - in number of inputs, number of neurons in hidden layer, PSO method used for training, and optimized objective function.

The architecture of the applied artificial neural network models is a multilayer perceptron with one input layer, one hidden layer of neurons, and one output layer with one output neuron. The topology is fully connected, and transfer of information is feedforward. The activation function of neurons is the RootSig.

The weights in ANN models were trained with 5 different PSO optimization techniques. As optimized objective criteria serve 5 different statistics, which are often used in hydrological modelling. For SPEI simulations, the integrated neural network models with different settings were used.

In the research, always 5 artificial neural network models were integrated into one hybrid ANN model (hANN). The outputs from four models are inputs into the fifth model as it is displayed on Figure 5.1. The final forecasted SPEI drought index is the output from the fifth ANN model.

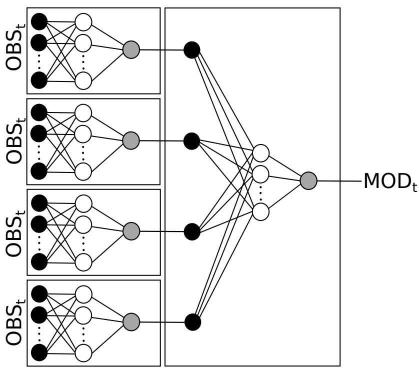

Figure 5.1: Integrated ANN models into hANN. Circles filled with black represent input layer, circles filled with white represent hidden layer, and circles filled with grey represent outputs

Table 5.1: The best levels of each factor for each accuracy criteria, and the final best level based on Tukey's HSD test. Minus sign indicates no significant difference in levels

Factor	**MSE**	**NS**	**PI**	**cAI1**	**cAI2**	**Final**
Calibration period						
Catch.	01371500	01371500	01197500	01197500	01371500	01371500
N_{in}	12, 12s	-	6	12, 12s	12, 12s	12, 12s
N_{hd}	6	6	6	6	6	6
OOF[a]	2, 3, 4, 5	-	1, 2, 4, 5	1, 2, 3, 5	1, 2, 3, 4	2
PSO[b]	-	5	5	-	-	5
Validation period						
Catch.	01445500	01503000	01127000	01372500	01445500	01445500
N_{in}	-	6	6	-	12, 12s	6
N_{hd}	6	6	6	6	-	6
OOF[a]	2, 3, 4, 5	-	-	1, 2, 3, 5	-	2, 3, 5
PSO[b]	-	4, 5	2, 3, 4, 5	-	-	4, 5

[a] $1 = MSE$, $2 = NS$, $3 = PI$, $4 = cAI1$, $5 = cAI2$

[b] $1 = LinPSO$, $2 = ChaoPSO$, $3 = NonlinPSO$, $4 = AdaptPSO$, $5 = APartPSO$

5.2 Results

The analysed catchment (Catch.), number of inputs (N_{in}), number of neurons in hidden layer (N_{hd}), optimized objective function (OOF), and PSO variant were considered as factors influencing the resulted accuracy criteria.

The best levels of each factor obtained during calibration and validation reflects Table 5.1. It is evident, that some levels are significantly better for simulations, but sometimes there is no difference between two or more levels. Based on the results, the best hANN models were determined. For calibration, there are two hANN models with two different N_{in} with the same simulation ability. The superior are 12 inputs into the neural networks with 6 neurons in the hidden layer optimized by Nash-Sutcliffe efficiency (NS) criteria with $APartPSO$ method. For validation, there exist six hANN models with three OOF and two PSO factors, whose performances are not different. The best results were obtained by models with 6 SPEI inputs and 6 neurons in the hidden layer.

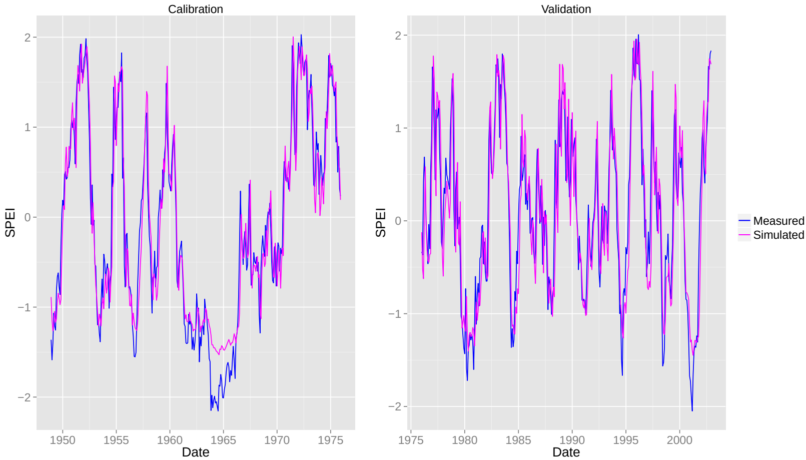

Figure 5.2: Measured and simulated time series of SPEI during calibration and validation period in the catchment 01371500 for the best hANN model 12-6-*APartPSO-NS*

Figure 5.2 presents the time series of measured and simulated SPEI drought index. The simulated SPEI is close to the measured one, and the model provides sufficient forecasts. Upon closer investigation, the best hANN obtained during calibration provides good fit also for validation data, and vice versa. The only problem could be the overestimation of the lower values of SPEI.

5.3 Conclusions

The main aim of this chapter was to combine hybrid neural network models with particle swarm optimization, which was used as training algorithm for the ANN weights.

In total, 150 hybrid ANN models were applied for simulating the SPEI drought index on 8 US catchments. The dataset of 54 years of observations was divided into calibration and validation period, and the performance was analysed based on five measures of goodness of fit.

It was found out that the number of neurons in hidden layer of the ANN models influences results the most. Better performance was achieved with 6 neurons in the hidden layer instead of 3. The best number of neurons in the input layer was not determined uniquely. For calibration, better results were obtained with 12 inputs, compared to 6 input variables for validation.

Even though, the results obtained by different PSO variants were not always statistically different, the *APartPSO* is the most effective method for SPEI forecasting. The choice of PSO variant was not essential in all cases, but the adaptive variants gave better results in both calibration and validation.

The best objective function optimized by the final ANN model is the NS. In all cases, more OOF gave similar results, but in final evaluation of the model performances, the Nash-Sutcliffe efficiency was the most effective.

The results of this study extended the range of utilization of the particle swarm optimization technique and artificial neural network modelling. The combination of ANN with PSO is suitable for forecasting the SPEI drought index, and can be used for prediction of the potential threat of drought event.

Chapter 6

Principal conclusions and summary

Finding the optimal state of reality is the main purpose of the optimization process. The best variant from many possibilities is selected, and the effectiveness of the given system increases. Optimization has been applied in many real life engineering problems as in hydrological modelling. Within the hydrological case studies, the optimization process serves to estimate the best set of model parameters, or to train model weights in artificial neural networks.

Due to difficulties, which may occur during optimization, it is necessary to wisely choose a suitable method. Based on the optimization problem, it is recommended to devote some time modifying the selected optimization method.

In this doctoral thesis, I focused on the particle swarm optimization technique, and its utilization in hydrological modelling. It is relatively recent optimization method, which has only a few parameters to adjust, and is easy to implement to the selected problem. The original algorithm was modified by many authors. They focused on changing the initialization of particles in the swarm, updating the population topology, adding new parameters into the equation, or incorporating shuffling mechanism into the algorithm.

The main goals of the thesis were provision of comprehensive review about the PSO method, implementation of selected PSO modifications together with a new proposed variant in C++ programming language, and application of the best modifications in real-life optimization problems from the field of hydrology.

The comprehensive review about the PSO technique was provided in Chapter 2. Due to the limited space in the thesis, I focused mainly on features, which were thereafter useful for my research. The original equations with different modifications were summarized there together with various topologies and applicable objective functions.

Comparison of selected PSO modifications was provided in Chapter 3. In total, 27 modifications were tested on 5 uni-modal and 6 multi-modal benchmark problems. Variants with constriction factor and different types of inertia weight were analysed. The results showed that the best PSO variant is the method with adaptive inertia weight parameter. In addition, the shuffled complex evolution strategy improved the performance, and gave the best results, which confirmed the usefulness of this approach. Therefore, I decided to later focus the attention to this direction of possible modifications, i.e. adaptive version of inertia weight, and sub-swarms with shuffling and redistribution of particles.

In Chapter 4, a new PSO variant was proposed. The method enhances the global exploration and local exploitation in the parametric space during the optimization process through new adaptive strategy of inertia weight. The shuffled complex evolution strategy was incorporated into the algorithm. The optimization ability of the proposed method was tested on 11 benchmark problems, and the obtained results were compared with 3 PSO modifications from Chapter 3. It was found out that the new proposed variant performs well, and has suitable results.

Due to the fact, that the new proposed PSO version achieved good results in optimizing benchmark functions, it was applied in two real-life optimization problems. One case study concerned with hydrological model Bilan (Chapter 4), and second case study dealt with artificial neural networks (Chapter 5).

The new method together with other 3 PSO modifications was used for finding the solution of inverse problems related to estimation of parameters of rainfall-runoff model Bilan (Chapter 4). Based on statistical tests, it was concluded that the best results were obtained by the new proposed method and by the adaptive variant, which was also the best method in Chapter 3. On the other hand, the PSO modification with parameter of constriction factor performed the worst, which is also in agreement with the findings of Chapter 3.

The 4 best PSO modifications from Chapter 3 together with the proposed method from Chapter 4 were combined with artificial neural networks in Chapter 5. The integrated hybrid models were used for forecasting the standardized precipitation evapotranspiration drought index. The influence of each PSO method and other variables on the simulations was analysed. The variable, which influenced the results the most, was number of neurons in hidden layer of the ANN models. Therefore, it is essential to choose the size of hidden layer appropriately. In terms of PSO method, the most effective technique for SPEI forecasting was the proposed variant from Chapter 4.

Based on the results obtained during my research, I can conclude that adaptive version of inertia weight parameter is the most effective approach from all analysed variants. The shuffled complex evolution also significantly improves the optimization. The new PSO method proposed in this thesis finds the optimum value not only in benchmark problems, but also in real-life optimization problems. Therefore, it can be applied in other engineering studies.

Overall, the contribution of the doctoral thesis for the current stage of scientific knowledge is evident from the individual chapters. The results of this thesis extended the utilization of PSO methods in real-life engineering optimization problems. All analysed PSO algorithms are available for later use, and the completed algorithms are basis for other research projects.

Chapter 7

Shrnutí

Hlavním cílem optimalizačního procesu je nalezení optimálního stavu dané reality. Z mnoha možností je vybrána nejlepší varianta, čímž vzroste efektivita celého systému. Optimalizační technika byla aplikována v mnoha inženýrských problémech. V rámci hydrologického modelování je využita k odhadu nejlepší sady parametrů modelu, či k trénování umělých neuronových sítí.

Relativně novou optimalizační metodou je optimalizace rojem částic (PSO), která se vyznačuje malým množstvím parametrů pro nastavení a jednoduchou implementací. Původní algoritmus této metody byl mnoha autory modifikován. Důraz byl kladen na změnu způsobu inicializace částic v hejnu, aktualizaci topologie populace, přidání nového parametru do rovnice, či začlenění mechanismu promíchávání do algoritmu.

Modifikace PSO algoritmu zlepší provedení optimalizace, zamezí předčasné konvergenci a sníží výpočetní čas systému. Z těchto důvodů zahrnují hlavní cíle předložené doktorské práce navržení nové modifikace PSO metody s její implementací v programovacím jazyce C++. V práci bylo porovnáno a vyhodnoceno více PSO variant a nejlepší metody byly použity ve dvou hydrologických případových studiích.

První případová studie se zabývá použitím PSO algoritmů na inverzních problémech spojených s odhadem parametrů srážko-odtokového modelu Bilan. Ve druhé studii byly zkombinovány umělé neuronové sítě s PSO metodou pro předpověď vybraného indexu sucha.

Bylo zjištěno, že optimalizace rojem částic je vhodným nástrojem pro řešení problémů v rámci hydrologického modelování. Nejefektivnějšími PSO modifikacemi jsou varianty s adaptivní verzí váhovacího faktoru, které aktualizují rychlost částice během prohledávání vícedimenzionální řešené oblasti pomocí zpětné vazby. Mechanismus promíchávání a přerozdělování částic do komplexů, ve kterých je samostatně spouštěn PSO algoritmus, také výrazně zlepšil provedení optimalizace.

Přínos této doktorské práce spočívá ve vytvoření nové PSO modifikace, která byla otestována na referenčních problémech a úspěšně aplikována ve dvou hydrologických případových studiích. Výsledky práce rozšířily využití PSO metody v reálných inženýrských problémech a všechny analyzované PSO algoritmy jsou k dispozici pro pozdější využití v rámci dalších výzkumných projektů.

Curriculum vitae

Ing. Michala Jakubcová

Personal information

Date of birth:	27 February, 1987
Place of birth:	Liberec, Czech Republic
Address:	Na Maninách 27, 170 00 Praha 7, Czech Republic
E-mail:	michala.jakubcova@gmail.com

Education

2011 - till now	Ph.D.; Faculty of Environmental Sciences, Czech University of Life Sciences Prague, study program: Environmental modeling
2013 – 2014	MSc.; Wageningen University (Netherlands), study program: Earth and Environment, specialisation: Hydrology and Water Resources (incomplete)
2009 – 2011	Ing.; Faculty of Environmental Sciences, Czech University of Life Sciences Prague, study program: Environmental modeling
2006 – 2009	Bc.; Faculty of Environmental Sciences, Czech University of Life Sciences Prague, study program: Applied ecology
1998 – 2006	Gymnasium U Balvanu, Jablonec nad Nisou

Employment

2014 – till now	Researcher; Department of Fluid Dynamics, Institute of Thermomechanics Academy of Sciences of the Czech Republic, v.v.i.

Language knowledge

Czech (native), English (C1), German (A1)

Teaching at the FES CULS Prague

Basics of the water management (CZ; practicals; 2011, 2012)
Small water reservoirs (CZ; practicals; 2012)
Hydrology (EN, CZ; practicals; 2012, 2014, 2015)
Air protection (CZ; practicals; 2013)
Hydraulics (EN; whole course; 2014)
Flow in atmospheric boundary layer (EN; whole course; 2015)

Participation on projects

2015 IGA, No 20154219	Particle swarm optimization v umělých neuronových sítích
2014 IGA, No 20144227	Aplikace metody particle swarm optimization v hydrologickém modelování
2013 IGA, No 20134271	Strategie sub-populací v optimalizační metodě particle swarm optimization
2012 IGA, No 20124259	Modifikace metody Particle Swarm Optimization

Publications

Peer-review papers in journals with impact factor:

JAKUBCOVÁ M., MÁCA P., AND PECH P., 2015 (submitted): Combination of hybrid artificial neural networks with particle swarm optimization algorithm for SPEI forecasting. *Applied Soft Computing*.

JAKUBCOVÁ M., MÁCA P., AND PECH P., 2015: Parameter estimation in rainfall-runoff modelling using distributed versions of particle swarm optimization algorithm. *Mathematical Problems in Engineering*, vol. 2015, Article ID 968067, 13 pp.

JAKUBCOVÁ M., MÁCA P., AND PECH P., 2014: A comparison of selected modifications of the particle swarm optimization algorithm. *Journal of Applied Mathematics*, vol. 2014, Article ID 293087, 10 pp.

Conference proceedings in SCOPUS and WoS:

JAKUBCOVÁ M., 2015: Using particle swarm optimization algorithm for parameter estimation in hydrological modelling. In: *GeoConference on informatics, geoinformatics and remote sensing*. SGEM2015 Conference Proceedings, Sofia, Bulgaria, Book 2, Vol. 1, p. 399-406.

JAKUBCOVÁ M., 2014: Modifications of the particle swarm optimization and new proposed variant. In: *GeoConference on informatics, geoinformatics and remote sensing*. SGEM2014 Conference Proceedings, Sofia, Bulgaria, Book 2, Vol. 1, p. 257-264.

NĚMEČKOVÁ M., 2013: How constrained space affects the results in the particle swarm optimization. In: *GeoConference on informatics, geoinformatics and remote sensing*. SGEM2013 Conference Proceedings, Sofia, Bulgaria, Vol. 1, p. 131-138.

Other conference proceedings:

NĚMEČKOVÁ M., 2012: Analýza vybraných modifikací metody Particle Swarm Optimization. In: *Sborník abstraktů z konference HYDROMODE 2012*. Kostelec nad Černými Lesy, p. 19.

NĚMEČKOVÁ M., 2012: A comparison of particle swarm optimization algorithms based on constrained and unconstrained area. In: *Sborník abstraktů z konference UCOLIS 2012*. Kostelec nad Černými Lesy, p. 19.

Bibliography

[1] ANGELINE, P. J. Using selection to improve particle swarm optimization. In *Proceedings of the 1998 IEEE International Conference on Evolutionary Computation* (Anchorage, AK, 1998), pp. 84–89.

[2] BLUM, C. Ant colony optimization: Introduction and recent trends. *Physics of Life Reviews 2*, 4 (2005), 353–373.

[3] BLUM, C., AND MERKLE, D. *Swarm Intelligence: Introduction and Application*. Springer, 2008.

[4] CLERC, M., AND KENNEDY, J. The particle swarm-explosion, stability, and convergence in a multidimensional complex space. *IEEE Transactions on Evolutionary Computation 6*, 1 (2002), 58–73.

[5] DERRAC, J., GARCÍA, S., MOLINA, D., AND HERRERA, F. A practical tutorial on the use of nonparametric statistical tests as a methodology for comparing evolutionary and swarm intelligence algorithms. *Swarm and Evolutionary Computation 1*, 1 (2011), 3–18.

[6] EBERHART, R., AND SHI, Y. Particle swarm optimization: developments, applications and resources. In *Proceedings of the 2001 Congress on Evolutionary Computation* (Seoul, 2001), vol. 1, pp. 81–86.

[7] GERSHENFELD, N. *The nature of mathematical modeling*. Cambridge University Press, 1999.

[8] KARABOGA, D. An idea based on honey bee swarm for numerical optimization. Tech. rep., Technical report-tr06, Erciyes university, Engineering faculty, Computer engineering department, 2005.

[9] KENNEDY, J., AND EBERHART, R. Particle swarm optimization. In *Proceedings of the 1995 IEEE International Conference on Neural Networks* (Perth, WA, 1995), pp. 1942–1948.

[10] KRISHNANAND, K., AND GHOSE, D. Detection of multiple source locations using a glowworm metaphor with applications to collective robotics. In *Swarm Intelligence Symposium, 2005. SIS 2005. Proceedings 2005 IEEE* (2005), IEEE, pp. 84–91.

[11] MAXWELL, I. Processing: Autonomous Steering Behaviours - Part 02. `http://www.supermanoeuvre.com/blog/?p=327`, 2009. Online, accessed 20. 5. 2013.

[12] MENDES, R. *Population topologies and their influence in particle swarm performance*. PhD thesis, University of Minho, 2004.

[13] MICHALEWICZ, Z., AND FOGEL, D. *How to Solve It: Modern Heuristics*. Springer, 2004.

[14] PARSOPOULOS, K. E., PLAGIANAKOS, V. P., MAGOULAS, G. D., AND VRAHATIS, M. N. *Advances in Convex Analysis and Global Optimization*. Springer, 2001, ch. Improving particle swarm optimizer by function stretching, pp. 445–457.

[15] PARSOPOULOS, K. E., AND VRAHATIS, M. N. *Advances in Intelligent Systems, Fuzzy Systems, Evolutionary Computation*. WSEAS Press, 2002, ch. Initializing the particle swarm optimizer using the nonlinear simplex method, pp. 216–221.

[16] REYNOLDS, C. W. Flocks, herds and schools: A distributed behavioral model. *SIGGRAPH Comput. Graph. 21*, 4 (1987), 25–34.

[17] SUGANTHAN, P. N., HANSEN, N., LIANG, J. J., DEB, K., CHEN, Y. P., AUGER, A., AND TIWARI, S. Problem Definitions and Evaluation Criteria for the CEC 2005 Special Session on Real-Parameter Optimization. Tech. rep., Nanyang Technological University, Singapore, 2005.

[18] WEISE, T. Global optimization algorithms-theory and application. *Self-Published,* (2009).

[19] WEISE, T., ZAPF, M., CHIONG, R., AND URBANEJA, A. J. Why Is Optimization Difficult? In *Nature-Inspired Algorithms for Optimisation*, R. Chiong, Ed., vol. 193 of *Studies in Computational Intelligence*. Springer, 2009, ch. 1, pp. 1–50.