

Shuffled Complex Evolution Metropolis (SCEM-UA) global optimization algorithm - Jasper Vrugt

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 Uncertainty Analysis in
 Environmental Modelling
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a) Introduction:

While considerable attention has been given to the development of automatic calibration methods which aim to successfully find a single best set of parameter values, much less attention has been given to a realistic assessment of parameter uncertainty in hydrologic models. Markov Chain Monte Carlo (MCMC) methods have become increasingly popular to estimate parameter uncertainty in the settings of a Bayesian framework. However, MCMC methods require the a-priori definition of a proposal or sampling distribution. The Shuffled Complex Evolution Metropolis (SCEM-UA) global optimization algorithm is a MCMC sampler which is well suited to infer the posterior probability distribution of hydrologic model parameters. The algorithm is a modified version of the original SCE-UA global optimization algorithm and operates by merging the strengths of the Metropolis algorithm, controlled random search, competitive evolution, and complex shuffling in order to continuously update the proposal distribution and evolve the sampler to the posterior target distribution.

b) Advantages

The method:

- Generates explicit estimates of parameter uncertainty in a single optimization run (so estimates the entire posterior parameter distribution);
- Generates prediction uncertainty bounds on the model simulations;
- Generates improved estimates of parameter sensitivity and correlation in the full parameter space. This information is very useful to estimate what complexity is warranted by the calibration data.
- Generates useful estimates of the most informative measurements and time varying parameters in recursive mode (PIMLI)

c) Disadvantages

- The method is computationally demanding, especially for high-dimensional state/parameter estimation problems;
- Method relies on correct model structure and Bayesian statistics.
- Method ignores input, output, and model structural uncertainty. In principle this could be incorporated in the identification procedure (see SODA);
- How to deal with soft data?

d) Assumptions

Uses classical Bayesian density functions to estimate model parameters (assuming model is correct and no input errors)

Fully based on Bayesian model identification

Model is available (based on a-prior information)

e) Most appropriate application areas

Watershed model calibration/evaluation

Subsurface hydrologic modeling/contaminant transport

Any field where modeling/measuring interface

f) Reading list

Vrugt, J.A., H.V. Gupta, W. Bouten, and S. Sorooshian, A Shuffled Complex Evolution Metropolis algorithm for optimization and uncertainty assessment of hydrologic model parameters, *Water Resour. Res.*, 39, 1201, doi:10.1029/2002WR001642, 2003.

Vrugt, J.A., H.V. Gupta, L. Bastidas, W. Bouten, and S. Sorooshian, Effective and efficient algorithm for multi-objective optimization of hydrologic models, *Water Resour. Res.*, 39, 1214, doi:10.1029/2002WR001746, 2003.

Vrugt, J.A., C.G.H. Diks, H.V. Gupta, W. Bouten, and J.M. Verstraten, Improved treatment of uncertainty in hydrologic modeling: combining the strengths of global optimization and data assimilation, In Press: *Water Resources Research*.

g) Software availability

Available in MATLAB and OCTAVE. Currently busy with implementation of SCEMUA, MOSCEM-UA, PIMLI and SODA on parallel grid computers.

h) Web links or other information

<http://staff.science.uva.nl/~jvrugt/>

http://www.science.uva.nl/ibed/research/Research_Fields/cbpg/products/

i) Figures

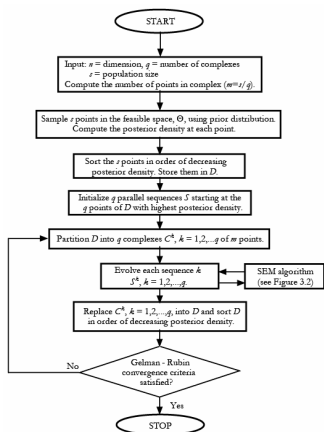


Figure 1. Flow chart of the SCEM-UA algorithm.

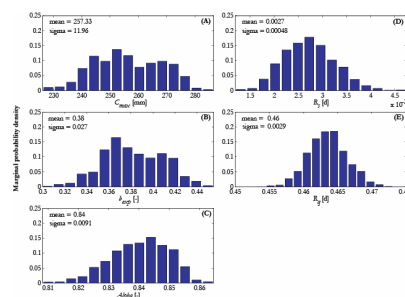


Figure 2. Marginal posterior probability distributions of the HYMOD model parameters constructed using 10,000 samples generated with the SCEM-UA algorithm and 3 years of daily streamflow data from the Leaf River in Mississippi. The HYMOD model prediction uncertainty ranges corresponding to this posterior pdf are presented in Figure 2b of the SODA poster.

j) Delegates Comments (please add !!)