The use of stochastic objective functions in water resource optimization problems

5th EGU Leonardo Conference – Hydrofractals 2013 – STAHY '13, Kos Island, Greece, 17–19 October 2013

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1. Abstract

Water resource problems are characterized by the presence of multiple sources of **uncertainty**. The implementation of **Monte Carlo simulation** techniques within powerful **optimization** methods are required, in order to handle such uncertainties. We investigate a modified version of the **evolutionary annealing-simplex** method in global optimization applications, where uncertainty is explicitly considered in terms of **stochastic objective functions**. We evaluate the algorithm against several **benchmark functions**, as well as in the **stochastic calibration** of a lumped rainfall-runoff model (Zygos). In this context, we investigate different calibration criteria and different sources of uncertainty, in order to assess not only the robustness of the derived parameters but also the predictive capacity of the models.

2. Optimization under uncertainty

Uncertainty appears in most of real-world optimization problems, including hydrological. Typical sources are: (a) **data uncertainty**, due to observation and processing errors; (b) **model uncertainty**, due to simplified representation of significantly complex systems; (c) **parameter uncertainty**, due to statistically inconsistent fitting criteria and inefficient calibrations.

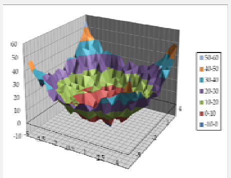

Fig. 1: Response surface of noisy sphere function $f(x_1, x_2) = x_1^2 + x_2^2 + N(0, 1)$.

The optimization problem under uncertainty can be formulated as:

$$\min f(\mathbf{x}) = \min F(\mathbf{x}, \omega), \ \mathbf{a} < \mathbf{x} < \mathbf{b}$$

where $\mathbf{x}$ is a vector of n control variables, $f(\mathbf{x})$ is the fitness function, ω is a noise component and $F(\mathbf{x}, \omega)$ a **random estimate** at $\mathbf{x}$. In the case of **simulation models**, where the system performance f is inferred either from historical or synthetic data samples, ω represents the **sampling uncertainty**. Uncertainty makes the response surface of the function even rougher, by randomly creating local minima and maxima (Fig. 1).

3. The modified evolutionary annealing-simplex (EAS) method for stochastic objective functions

EAS is a **heuristic global optimization** technique coupling the strength of simulated annealing in rough search spaces with the efficiency of the downhill simplex method (Nelder & Mead, 1965) in smoother spaces (Efstratiadis & Koutsoyiannis, 2002). Key features are:

- an **adaptive annealing cooling schedule** determines the degree of randomness through the search procedure;
- all transitions are probabilistic, since a stochastic term is added to the objective function, relative to **temperature**, thus $g(\mathbf{x}) = f(\mathbf{x}) + u\,T$;
- new points are generated via **simplex transformations** or **mutations**;
- all simplex configurations employ **quasi-stochastic scale factors**;
- **multiple expansions** and **uphill transitions** are allowed, in order to accelerate the search and escape from local minima, respectively.

The original version of EAS was modified to handle uncertain functions and avoid early convergence to local minima, due to the dominance of noise. These modifications include:

- **Dynamic adjustment of shrinkage** coefficient, based on T, which protects from an early degeneration of the simplex (Fig. 2).
- **Re-evaluation of the current best point** in the population after n subsequent transformations that reduce the simplex size; this ensures that search will be not guided by a point, in which was assigned an erroneously low value, due to noise.
- **Re-annealing** of the system when T becomes lower than a threshold, to enhance the search procedure with sufficient randomness.

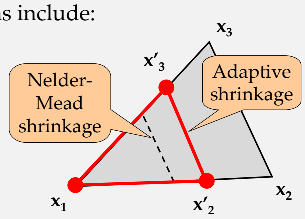

Fig. 2: Shrinkage of the simplex around the current best vertex $\mathbf{x}_1$ according to the Nelder-Mead formula, i.e. $\mathbf{x}'_i = 0.5\,(\mathbf{x}_i + \mathbf{x}_1)$ and the dynamic adjustment formula, given by $\mathbf{x}'_i = \delta\,\mathbf{x}_i + (1 - \delta)\,\mathbf{x}_1$, where $\delta = 1 - 0.5\,(T - T_0)$, T is the current temperature and T_0 is the initial temperature.

The new version of EAS is available in **R** (itia.ntua.gr/en/softinfo/29).

4. Mathematical applications

We tested six benchmark functions of ranging complexity in deterministic and stochastic setting, assuming three levels of Gaussian noise, $N(0.0, 0.75)$, $N(0.0, 1.0)$ and $N(0.0, 1.25)$. In all cases the global minimum lies in the origin ($\mathbf{x}^* = \mathbf{0}$).

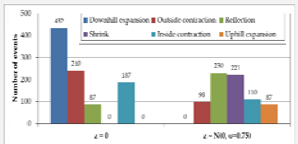

Fig. 4: Number of simplex moves in optimizing the deterministic and the noisy sphere function.

For each test function we carried out 100 independent runs of EAS, for $n = 2$ and $n = 10$ variables, as well as three population sizes (n+1, 2n+1, 8n+1). The results are summarized in Fig. 3. As shown in Fig. 4, the presence of uncertainty changes radically the optimization strategy, by favouring transitions that decrease the size of the simplex, which provides flexibility in highly non-convex spaces.

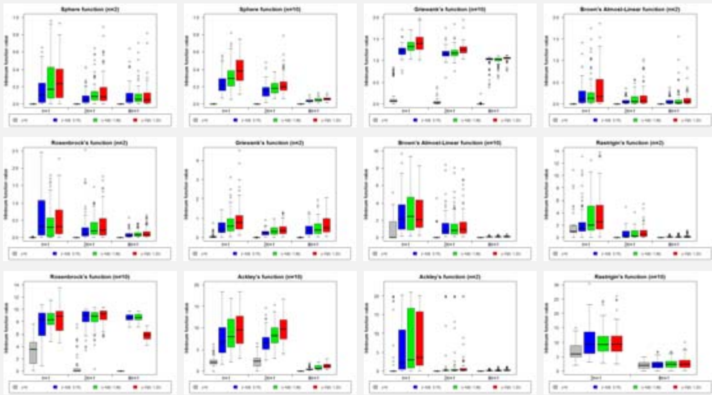

Fig. 3: Box plots with optimization results, derived from 100 runs for each problem.

5. Stochastic calibration of hydrological models

It is well-known that the parameters of conceptual hydrological models may vary substantially across different calibration periods. This questions **model transposability in time**, which is key requirement for ensuring a satisfactory **predictive capacity** (Gharari *et al.*, 2013).

In this context, we propose a stochastic calibration procedure, in which the fitting criterion (e.g. Nash-Sutcliffe efficiency, NSE) is estimated from **randomly changing samples** that are determined by means of (typically short) **moving windows** across the full series of the observed responses.

The above strategy was tested in three large-scale river basins of Greece (Acheloos, Aliakmon, Boeoticos Kephisos) that exhibit different hydrological behaviour, where we fitted the conceptual model **Zygos** against the observed runoff. The software supports various parameterizations, according to the complexity of each basin and the available data; its full structure uses nine parameters (http://itia.ntua.gr/en/softinfo/22).

We applied the EAS algorithm to provide 100 independent stochastic calibrations at each basin, with different moving windows. As shown in Fig. 5, even when using very short windows (i.e. from 1 to 5 years), the NSE values are close to the ones estimated from the full sample of observed runoff.

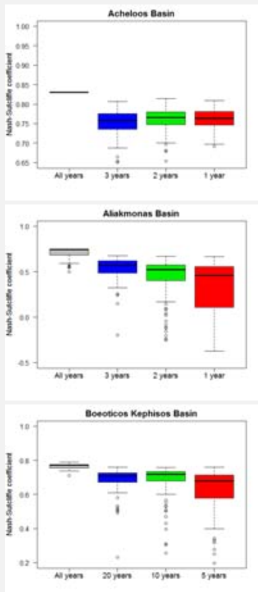

Fig. 5: Box plots of NSE at the three study basins, for different moving windows.

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