The multiobjective evolutionary annealing-simplex method and its application in calibrating hydrological models

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Hydrological modelling and multiobjective parameter estimation: The motivation

- Complex (semi- or fully-distributed) models generate multiple output variables at various sites → need for faithful reproduction of all model responses, that are representative of the watershed behaviour
- Due to the large number of parameters and their highly nonlinear interactions, alternative sets with similarly good performance may be detected (the “equifinality” problem) → need for establishment of “behavioural” (i.e., realistic, reliable and stable) parameter sets
- Models are too weak against data and structural errors → need to assess the sensitivity of parameters and the model predictive uncertainty
- Multiple error measures, when aggregated to a single objective function, formulate response surfaces that are strongly related to the aggregation scheme → need to distinguish the optimisation criteria, to avoid scaling problems and to investigate possible contradictory interactions
- Automatic calibration methods, involving too extended, high-dimensional and non-convex search spaces, are easily trapped by local optima or other peculiarities → need for reducing the parameter boundaries, to assist the searching procedure
Multiobjective optimisation: The story so far

- **“Philosophical” foundation (1880-1900):** the concept of Pareto-Edgeworth optimum, applied in sociology and welfare economics
- **Mathematical foundation (1950-1960):** formulation of the vector maximum problem by Kuhn and Tucker and first engineering applications
- **Plain aggregating approaches (1970):** a priori definition of the best compromise decision set, through the formulation of utility functions based on weighting coefficients, articulation of preferences, goal-vectors, etc.
- **Population-based non-Pareto approaches (1980):** formulation of sub-sets, each one evaluated according to different criterion (by switching objectives), and next shuffled and evolved through crossover and mutation (VEGA)
- **Dominance-based evolutionary approaches (1990):** use of ranking procedures, based on the principle of Pareto optimality, and techniques to maintain diversity through fitness sharing, to generate representative trade-offs among conflicting objectives (MOGA, NSGA, NPGA)
- **Modern approaches:** revision of multiobjective evolutionary schemes, with emphasis on efficiency, using faster ranking techniques, clustering methods and elitism mechanisms (SPEA, SPEA-II, NSGA-II, PAES, MOMGA, etc.)

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Multiobjective evolutionary algorithms: General principles

1. According to the principle of dominance, a rank measure \( r_i \) is assigned to each individual or group of individuals, where the best (lower) value corresponds to non-dominated points, thus guiding the search towards the Pareto front; a variety of rank values protects from high selection pressure.
2. A density measure \( \sigma_i \) is assigned to individuals, using sharing functions or nearest neighbour techniques, to maintain diversity within population, thus favouring the generation of well-distributed sets.
3. The selection process is implemented applying typical mechanisms (e.g., roulette, tournament), on the basis of dummy fitness of the form \( \phi_i = \phi(r_i, \sigma_i) \).
4. The evolution process is implemented using the typical genetic operators.

In multiobjective evolutionary search, due to the use of the concept of dominance in fitness evaluation, a discrete response surface is created, which is reformed at each generation.

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Applying multiobjective evolutionary algorithms for model calibration: Some drawbacks

- Search is computationally demanding, especially in the case of complex models with many parameters.
- There is too little experience regarding problems with more than two criteria.
- Fitting criteria are conflicting only in case of ill-posed structures or data.
- The concept of dominance is not necessarily consistent with the concept of “equifinality”; hence multiobjective search may result to non-behavioural, albeit Pareto optimal, parameter sets, providing extreme performance, i.e. too good against some criteria, too bad against the rest ones.
- A best-compromise parameter set is required for operational purposes.

The multiobjective evolutionary annealing-simplex (MEAS) method

**Phase 1: Evaluation**

A performance measure (fitness) is assigned, consisting of:
- a **rank measure**, based on a strength-Pareto scheme, which both ensures convergence to the real Pareto front and diversity preservation;
- an **indifference measure** for further discrimination of indifferent solutions in case of multiple (more than two) objectives;
- a **feasibility measure**, for guiding search toward a desirable region of the Pareto front, thus providing acceptable trade-offs among conflicting objectives.

**Phase 2: Evolution**

Evolution is implemented according to transition rules that are based on a simplex-annealing approach, where:
- a **downhill simplex pattern**, combining both deterministic and stochastic transition rules, is employed for offspring generation;
- an **adaptive annealing cooling schedule** is used to control the degree of randomness during evolution.
The MEAS method: Fitness assignment through a strength-Pareto approach

- The concept is based on the SPEA and SPEA-II methods (Zitzler and Thiele, 1999; Zitzler et al., 2002).
- For each individual, both dominating and dominated points are taken into account.
- Formulates a integral response surface that changes whenever a new individual is generated.
- Provides a large variety of rank values (larger than any other known ranking algorithm), as well as a sort of "nicching" mechanism, to preserve population diversity.
- A non-integral term is added to fitness, to penalise individuals excelling in fewer criteria than other indifferent ones, with identical rank.

Rank = sum strength of all dominators
Strength = number of dominated individuals

Non-dominated individuals have zero rank

The MEAS method: Restricting the feasible objective space

- Based on a concept inspired from the goal-programming method.
- Requires the specification of a constraint vector \( \mathbf{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_m) \) denoting the boundaries of a desirable ("feasible") region of the objective space.
- Ensures a better insight on the most promising parts of the Pareto front, where the best-compromise parameter set is suspected to be sited.

Computational steps
1. The maximum fitness value is computed, i.e. \( \Phi = \max \varphi(i) \).
2. Each individual \( i \) is checked whether it lies within the feasible space; if \( x_j > \varepsilon_j \) for the \( j \)th criterion, a square distance penalty \( \Delta \varepsilon_j = (x_j - \varepsilon_j)^2 \) is added to \( \varphi(i) \).
3. All infeasible individuals are further penalised by adding \( \Phi \); hence, they become worse than any other feasible individual, either dominated or not.
The MEAS method: A selection procedure based on a simulated annealing strategy

- Dominance term, $\varphi(i)$
- Feasibility term, $p(i)$
- Unit random number, $r$
- Current system's temperature, $T$

- Deterministic component, $y(i)$
- Stochastic component, $s(i)$

- Penalty measure

$$f(i) = \varphi(i) + p(i) + r \, T$$

Favours the survival of feasible and non-dominated solutions

Provides flexibility, to escape from local optima and handle peculiarities of non-convex spaces

The MEAS method: Evolving population

1. According to an **elitism** concept, the population is divided to non-dominated ($\varphi < 1$) and dominated ($\varphi > 1$) individuals.
2. The system **temperature** is regulated in order to not exceed $T_{\text{max}} = \xi \, \Delta y$, where $\xi \geq 1$ parameter of the annealing cooling schedule and $\Delta y$ the difference between the best and worst fitness of current population.
3. From the entire population $n + 1$ points are picked up, thus forming a **simplex** in the $n$-dimensional search space; at least one simplex vertex is selected from the dominated set, given that the latter is not empty.
4. The "weakest" individual $w$ is detected by means of maximisation of $f$.
5. A **crossover** scheme is employed on the basis of a downhill simplex pattern; if a better point $x'$ ("offspring") is located, it replaces $w$ and the temperature is reduced by $\lambda$, where $\lambda < 1$ parameter of the annealing cooling schedule.
6. If recombination fails (i.e., any better solution cannot be found), the offspring is generated via a random perturbation (**mutation**) of $w$, i.e. $x' = w + \Delta x$.

For an earlier, single-objective implementation of the evolutionary annealing-simplex method see: Efstratiadis and Koutsoyiannis (2002), Rozos et al. (2004)
The MEAS method: Simplex configurations

- Weakest vertex, \( w \)
- Centroid
- Reflection
- Outside contraction
- Offspring, \( x' \)
- Multiple expansion (one-dimensional minimisation)

Performance assessment of MEAS method:
Test function SCH-2

- Taken from Schaffer (1984)
- Single control variable, in the range [-100, 100]
- Extended feasible objective space
- Disconnected Pareto set (1 \( \leq \) \( x \) \( \leq \) 2 and 4 \( \leq \) \( x \) \( \leq \) 5)
- Disconnected and convex Pareto front
- Population size = 100
- Convergence to a non-dominated set after 9366 function evaluations
Performance assessment of MEAS method:
Test function KUR

- Taken from Kursawe (1991)
- 3 control variables, in the range [-5, 5]
- Non-convex Pareto front
- Population size = 100
- Convergence to a non-dominated set after 37563 function evaluations

Performance assessment of MEAS method:
Test function POL

- Taken from Poloni (1997)
- Two control variables, in the range \([-\pi, \pi]\)
- Non-convex and disconnected Pareto front
- Population size = 100
- Convergence to a non-dominated set after 2218 function evaluations
Performance assessment of MEAS method:
Test function ZDT-2

- Taken from Zitzler et al. (2000)
- 30 control variables, in the range [0, 1]
- Pareto set: 0 ≤ x₁ ≤ 1 and xᵢ = 0, for i = 2, ..., 30
- Non-convex Pareto front
- Population size = 100
- Convergence to a locally non-dominated set after 16080 function evaluations
- Final set obtained after 25000 function evaluations

Performance assessment of MEAS method:
Test function ZDT-3

- Taken from Zitzler et al. (2000)
- 10 control variables, in the range [0, 1]
- Disconnected Pareto set: 0 ≤ x₁ ≤ 1 and xᵢ = 0, for i = 2, ..., 10
- Convex and disconnected Pareto front
- Population size = 100
- Convergence to a non-dominated set after 12944 function evaluations
Performance assessment of MEAS method: Test function ZDT-6

- Taken from Zitzler et al. (2000)
- 10 control variables, in the range [0, 1]
- Pareto set: \(0 \leq x_i \leq 1\) and \(x_i = 0\), for \(i = 2, \ldots, 10\)
- Non-convex and non-uniformly distributed Pareto front
- Population size = 100
- Final set, with satisfactory spread of non-dominated points, found after 150000 function evaluations

Multiobjective calibration of a complex hydrological model: Study area

- Watershed area \(\sim 2000\) km\(^2\), with highly non-linear interactions between surface and groundwater processes and man-made interventions.
- Main modelling issues:
  - a semi-distributed schematisation of the hydrographic network;
  - a conceptualisation of surface processes, based on spatial elements with homogenous characteristics (hydrological response units, HRU) and fitting to each one a soil moisture accounting model of six parameters;
  - a multi-cell groundwater scheme, with two parameters assigned to each cell;
  - a water management model, estimating the optimal system fluxes (flows, abstractions).
- Model components: 5 sub-basins, 6 HRU, 35 groundwater cells
Multiobjective calibration of a complex hydrological model: Main assumptions

- **Observed series**: daily discharge measurements at the basin outlet (Karditsa tunnel), sparse (1-2 per month) discharge measurements at six main karstic springs, contributing more than 50% of total runoff
- **Control period**: October 1984-September 1990 (calibration period), October 1990-September 1994 (validation period)
- **Calibration criteria**: determination coefficients of monthly discharge series at the basin outlet and the main spring sites (*number of objectives = 7*)
- **Control variables**: soil moisture capacity ($K_i$) and recession rate for percolation ($\mu_i$), assigned to each HRU, conductivity ($C_i$) of each virtual cell that represents spring dynamics (*search space dimension = 18*)
- **Feasible search space**: $0 < K_i < 1000$ (in mm), $0 < \mu_i < 1$ (dimensionless), $0.000001 < C_i < 0.5$ (in m/s)
- **Algorithmic inputs**: sample size = 50, maximum function evaluations = 5000
- **Other model parameters**: obtained through an earlier single-objective optimisation scenario, based on a weighted objective function and handled by combining automatic and manual calibration methods (*Rozos et al., 2004*)

Multiobjective calibration of a complex hydrological model: Characteristic trade-offs

Trade-offs represent: (a) **modelling errors** due to the complexity of processes (negative correlation of some spring hydrographs with precipitation); and (b) **data errors**, due to the construction of control series based on few observations
Multiobjective calibration of a complex hydrological model: Restricting the objective space

Concluding remarks

- Despite the impressive progress of last years regarding the development of evolutionary multiobjective optimisation techniques, **limited experience** exist on operational applications of hydrological interest, and most of them restricted to two-dimensional objective spaces.
- When fitting hydrological models on numerous observed responses, **irregular Pareto fronts** are formed due to structural and data errors.
- In case of complex, ill-posed hydrological models with many parameters, a **multiobjective calibration approach** is necessary to:
  - reduce uncertainties regarding the parameter estimation procedure;
  - investigate acceptable trade-offs between optimisation criteria;
  - guide the search towards promising areas of both the objective and the parameter space.
- The **MEAS algorithm** is an innovative scheme, suitable for challenging hydrological calibration problems, which combines: (a) a fitness evaluation procedure based on a strength-Pareto approach and a feasibility concept, (b) an evolving pattern based on the downhill simplex method, and (c) a simulated annealing strategy, to control randomness during evolution.
References


This presentation is available on-line at:
http://itia.ntua.gr/e/docinfo/644

Poster presentation of the hydrological model:
Friday, 29 April 2005, 17:30 - 19:00, area Z028

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