European Geosciences Union (EGU) - General Assembly
Vienna, Austria, 25 - 29 April 2005
Session HS1: Hydroinformatics

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

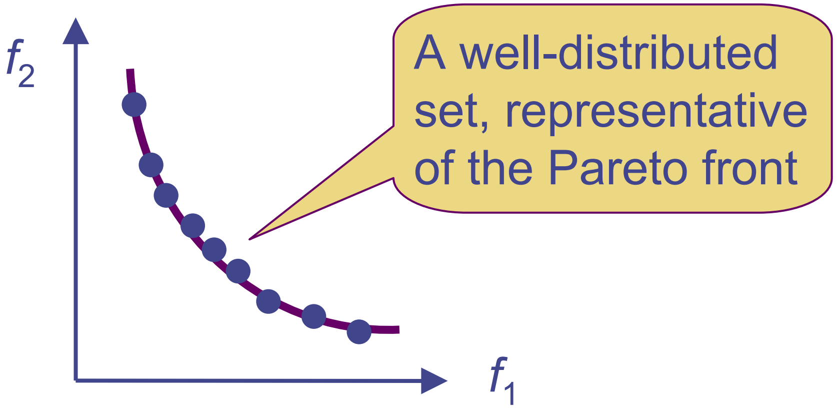
- Complex (semi- or fully-distributed) models generate multiple output variables at various sites → **need for faithful reproduction of all model responses, that are representative of the watershed behaviour**
- Due to the large number of parameters and their highly nonlinear interactions, alternative 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.)

Multiobjective evolutionary algorithms: General principles

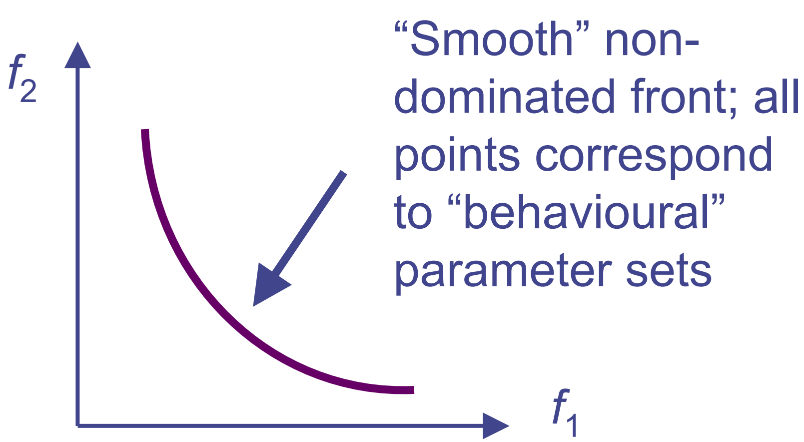
1. According to the principle of dominance, a **rank measure** r_i is assigned to each individual or group of individuals, where the best (lower) value corresponds to non-dominated points, thus guiding the search towards the Pareto front; a variety of rank values protects from high selection pressure.
2. A **density measure** σ_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 $\varphi_i = \varphi(r_i, \sigma_i)$.
4. The **evolution process** is implemented using the typical genetic operators.

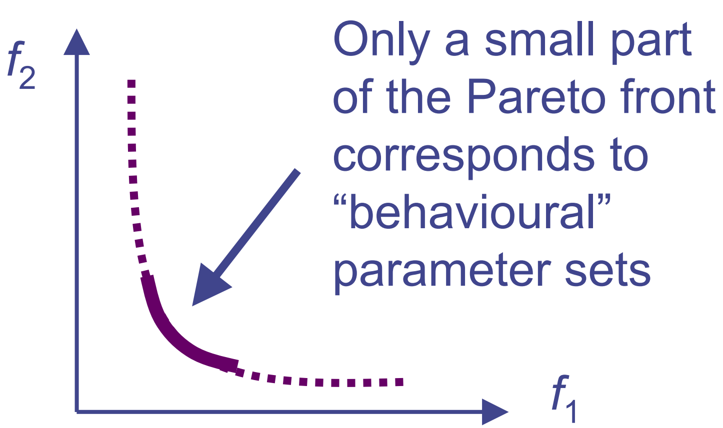


In multiobjective evolutionary search, due to the use of the concept of dominance in fitness evaluation, a **discrete response surface** is created, which is reformed at each generation.

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.

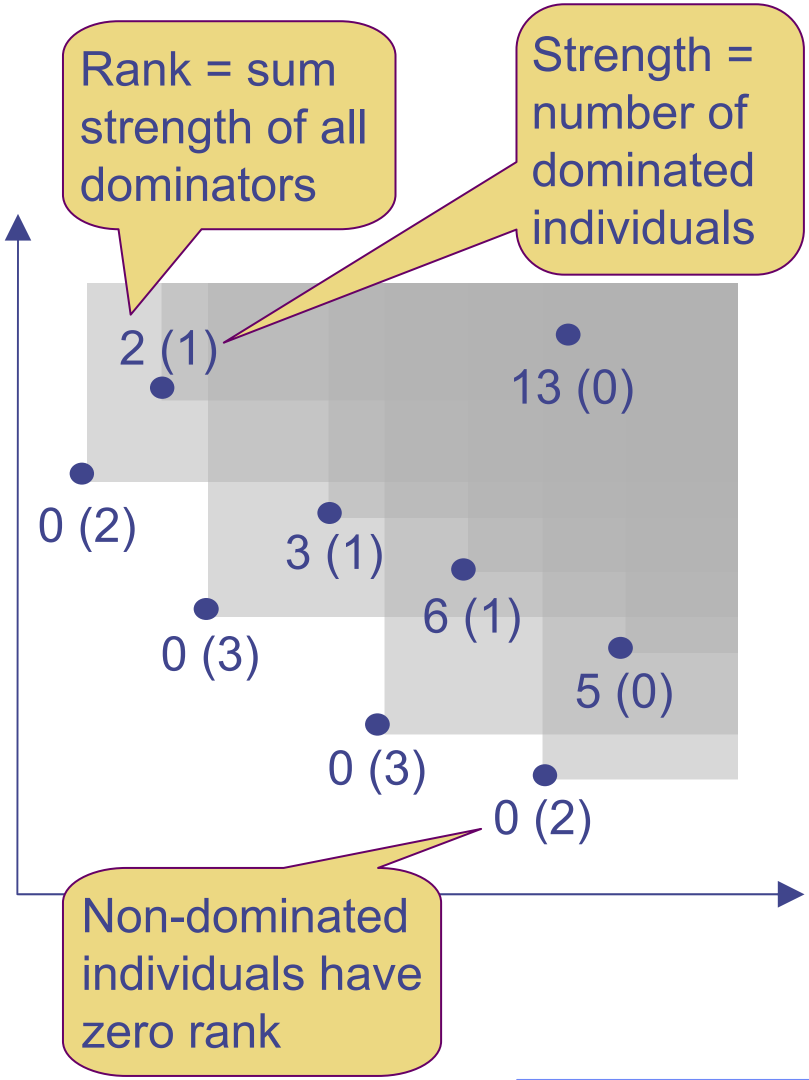
Phase 2: Evolution

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.

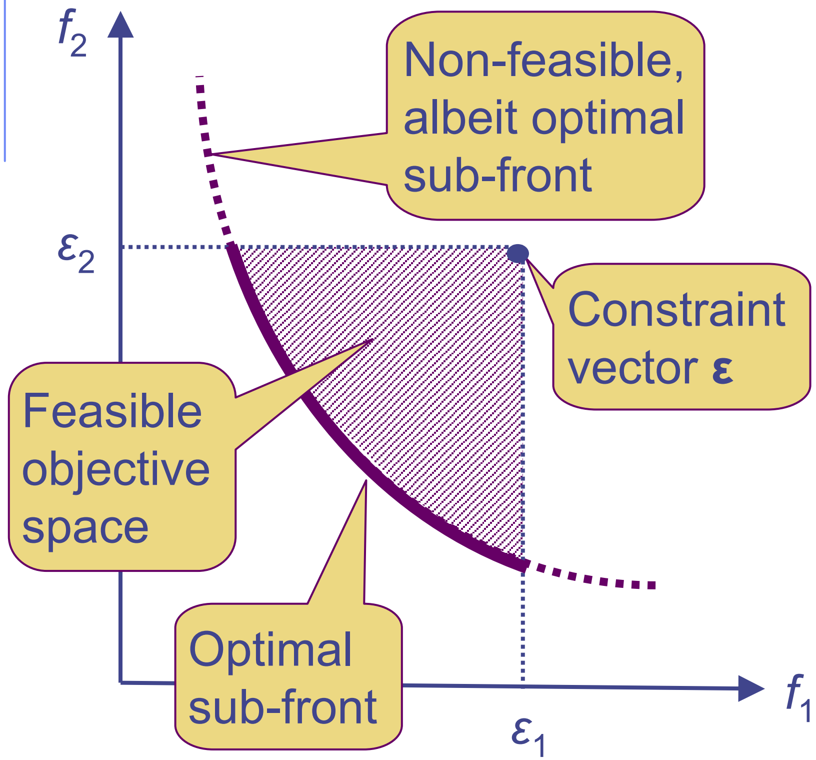
The MEAS method: Fitness assignment through a strength-Pareto approach

- 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 “niching” 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



The MEAS method: Restricting the feasible objective space

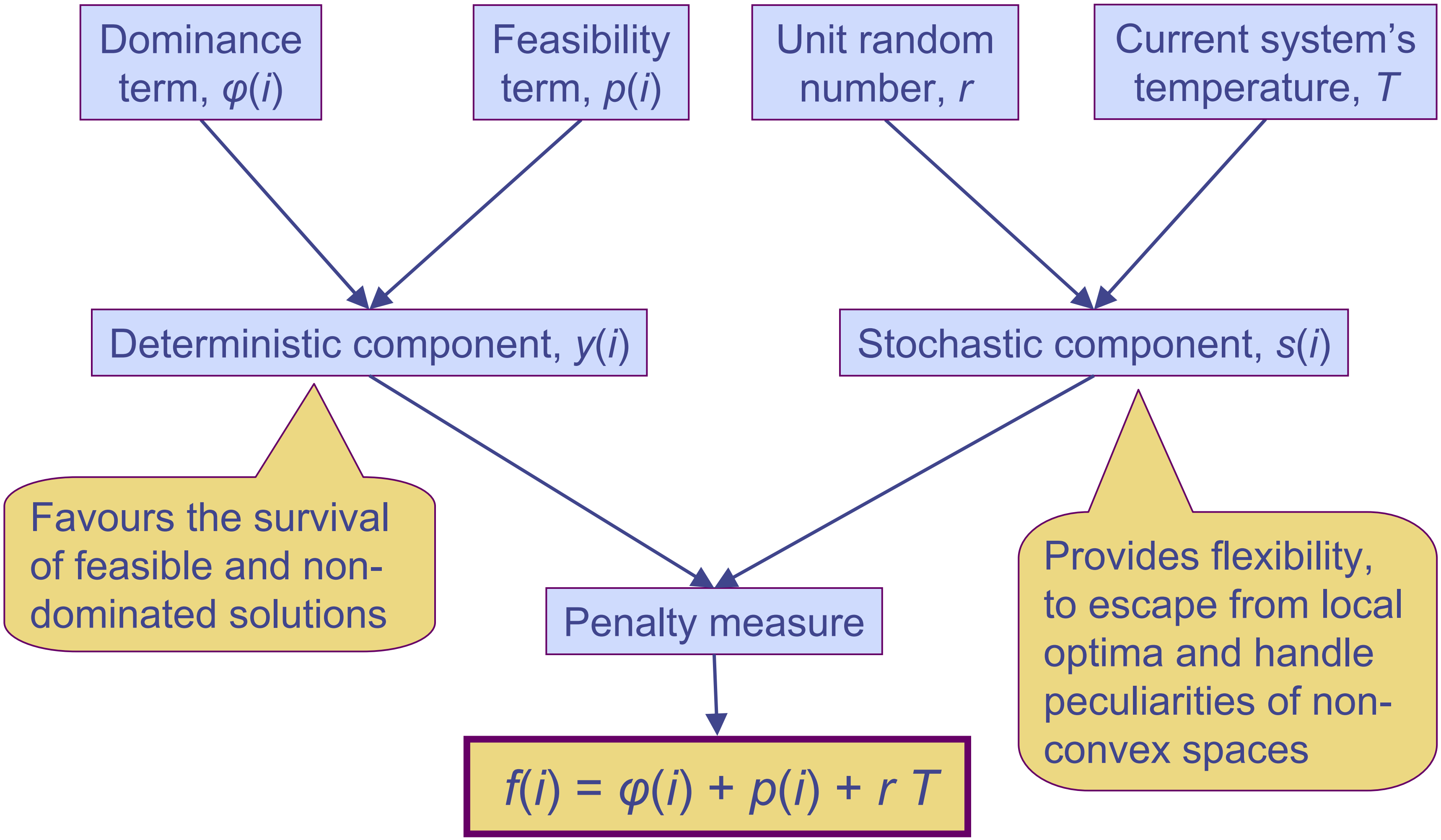
- Based on a concept inspired from the goal-programming method.
- Requires the specification of a constraint vector $\boldsymbol{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_m)$ denoting the boundaries of a desirable ("feasible") region of the objective space.
- Ensures a better insight on the 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 $x_{ij} > \varepsilon_j$ for the jth criterion, a square distance penalty $\Delta\varepsilon_{ij} = (x_i - \varepsilon_i)^2$ is added to $\varphi(i)$.
3. All infeasible individuals are further penalised by adding Φ; 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

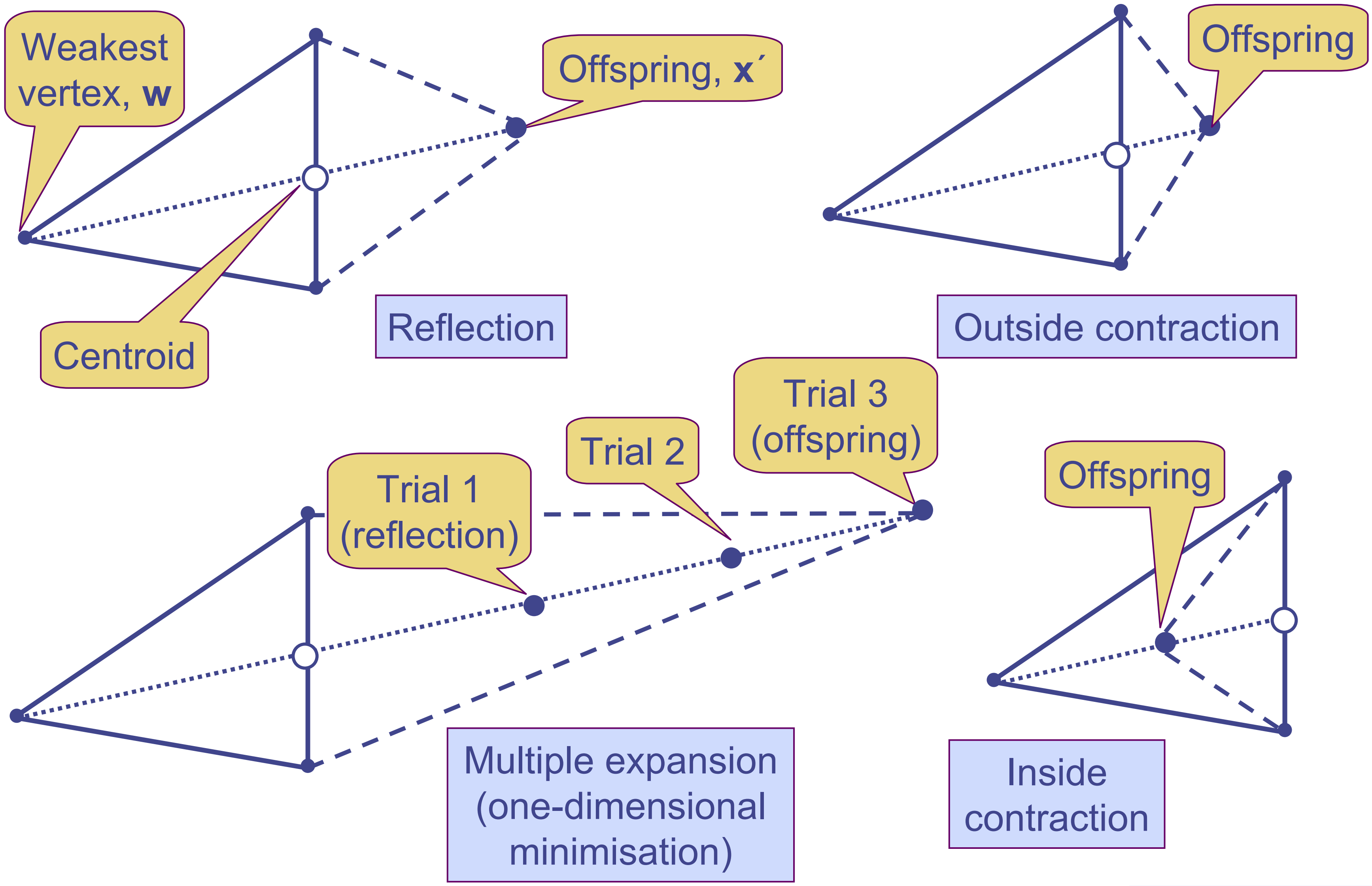


The MEAS method: Evolving population

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 $T_{max} = \xi\, \Delta y$, where $\xi \geq 1$ parameter of the annealing cooling schedule and Δy 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 λ, 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. $\mathbf{x}' = \mathbf{w} + \Delta\mathbf{x}$.

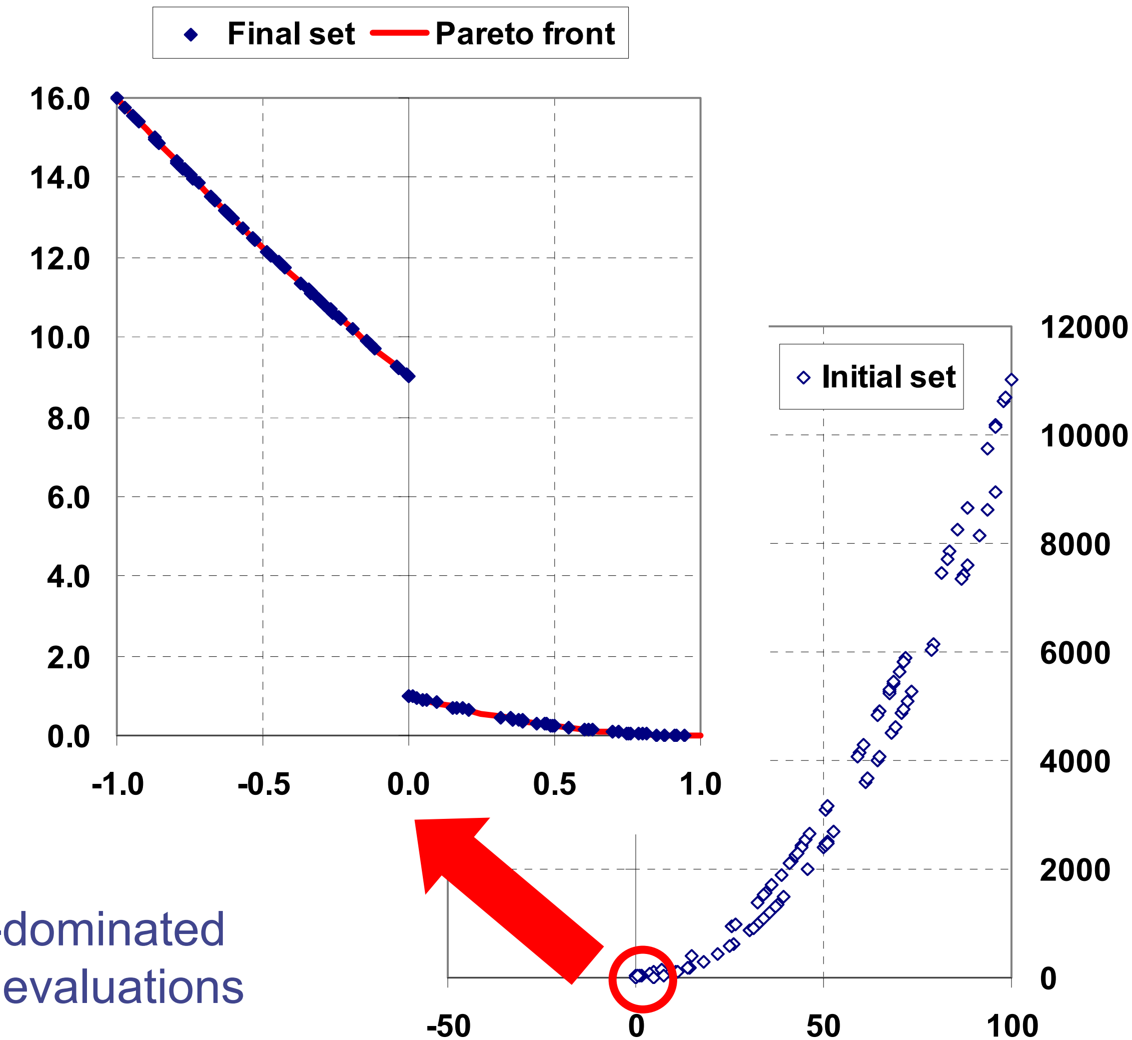
For an earlier, single-objective implementation of the evolutionary annealing-simplex method see: *Efstratiadis and Koutsoyiannis* (2002), *Rozos et al.* (2004)

The MEAS method: Simplex configurations



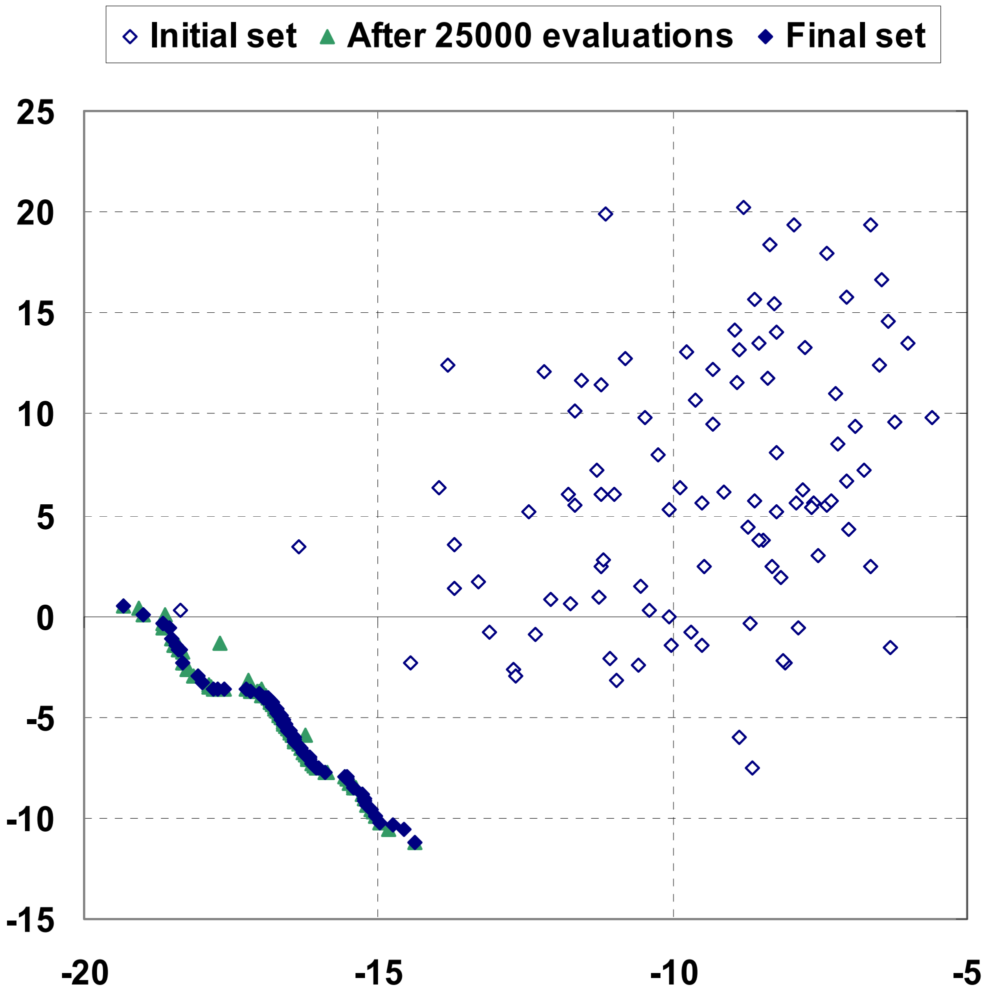
Performance assessment of MEAS method: Test function SCH-2

- Taken from *Schaffer* (1984)
- Single control variable, in the range [-100, 100]
- Extended feasible objective space
- Disconnected Pareto set (1 ≤ *x* ≤ 2 and 4 ≤ *x* ≤ 5)
- Disconnected and convex Pareto front
- Population size = 100
- Convergence to a non-dominated set after 9366 function evaluations



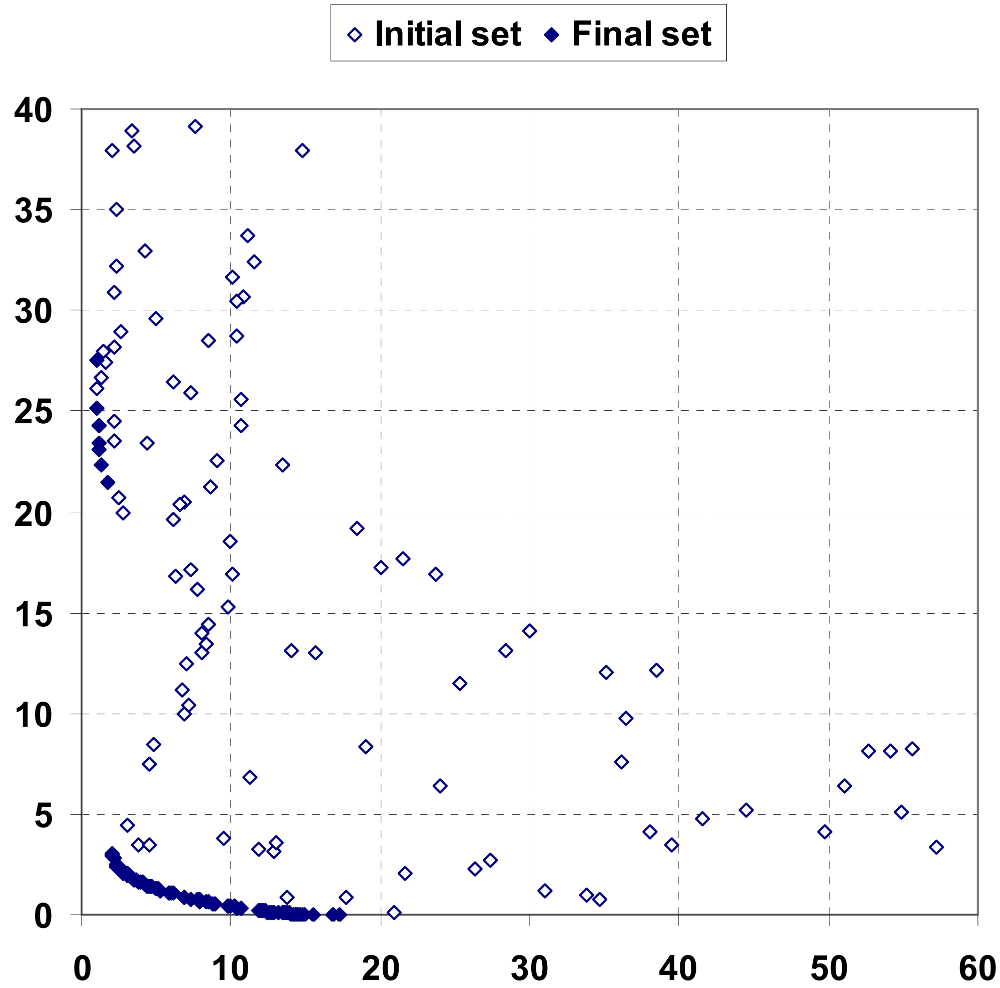
Performance assessment of MEAS method: Test function KUR

- 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



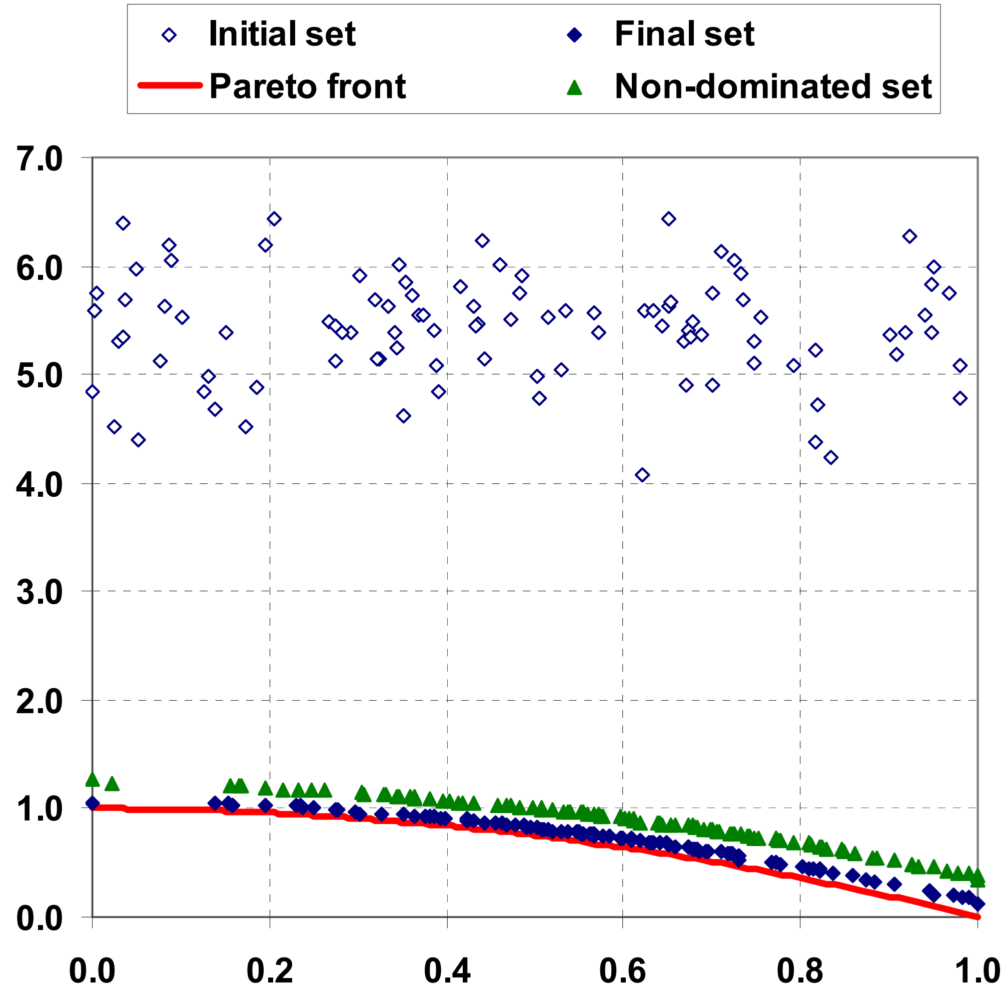
Performance assessment of MEAS method: Test function POL

- Taken from *Poloni* (1997)
- Two control variables, in the range [-π, π]
- Non-convex and disconnected Pareto front
- Population size = 100
- Convergence to a non-dominated set after 2218 function evaluations



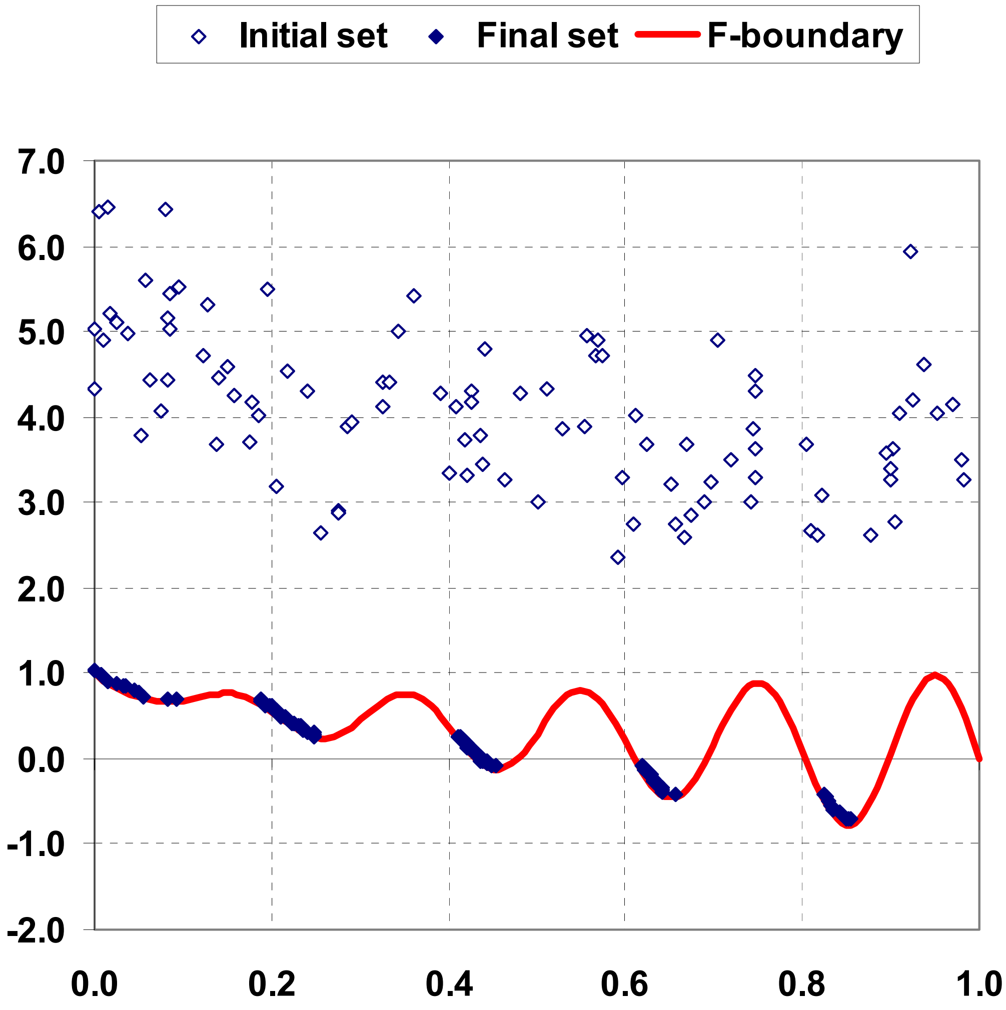
Performance assessment of MEAS method: Test function ZDT-2

- Taken from *Zitzler et al.* (2000)
- 30 control variables, in the range [0, 1]
- Pareto set: $0 \leq x_1 \leq 1$ and $x_i = 0$, 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



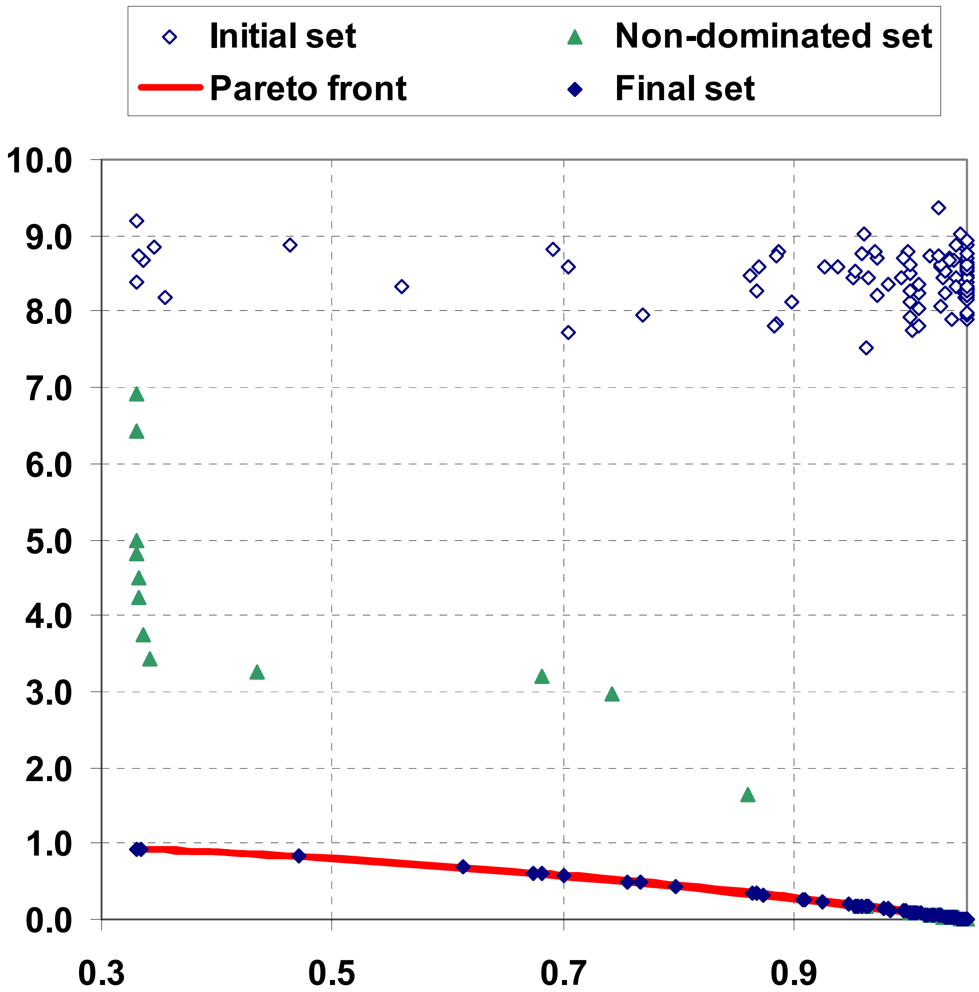
Performance assessment of MEAS method: Test function ZDT-3

- Taken from *Zitzler et al.* (2000)
- 10 control variables, in the range [0, 1]
- Disconnected Pareto set: $0 \leq x_1 \leq 1$ and $x_i = 0$, for $i = 2,..., 10$
- Convex and disconnected Pareto front
- Population size = 100
- Convergence to a non-dominated set after 12944 function evaluations



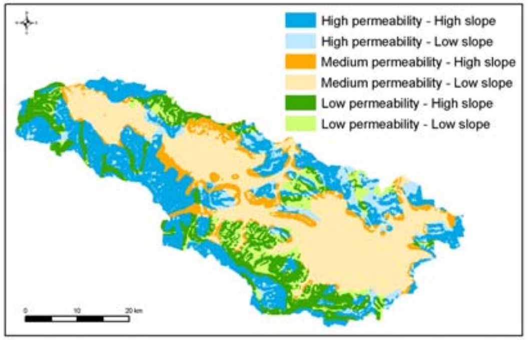
Performance assessment of MEAS method: Test function ZDT-6

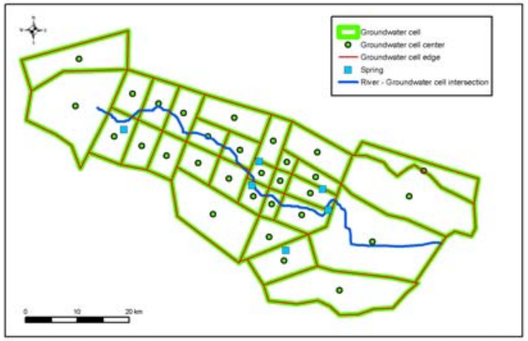
- Taken from *Zitzler et al.* (2000)
- 10 control variables, in the range [0, 1]
- Pareto set: $0 \le x_1 \le 1$ and $x_i = 0$, for $i = 2,.., 10$
- Non-convex and non-uniformly distributed Pareto front
- Population size = 100
- Final set, with satisfactory spread of non-dominated points, found after 150000 function evaluations



Multiobjective calibration of a complex hydrological model: Study area

- Watershed area ~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

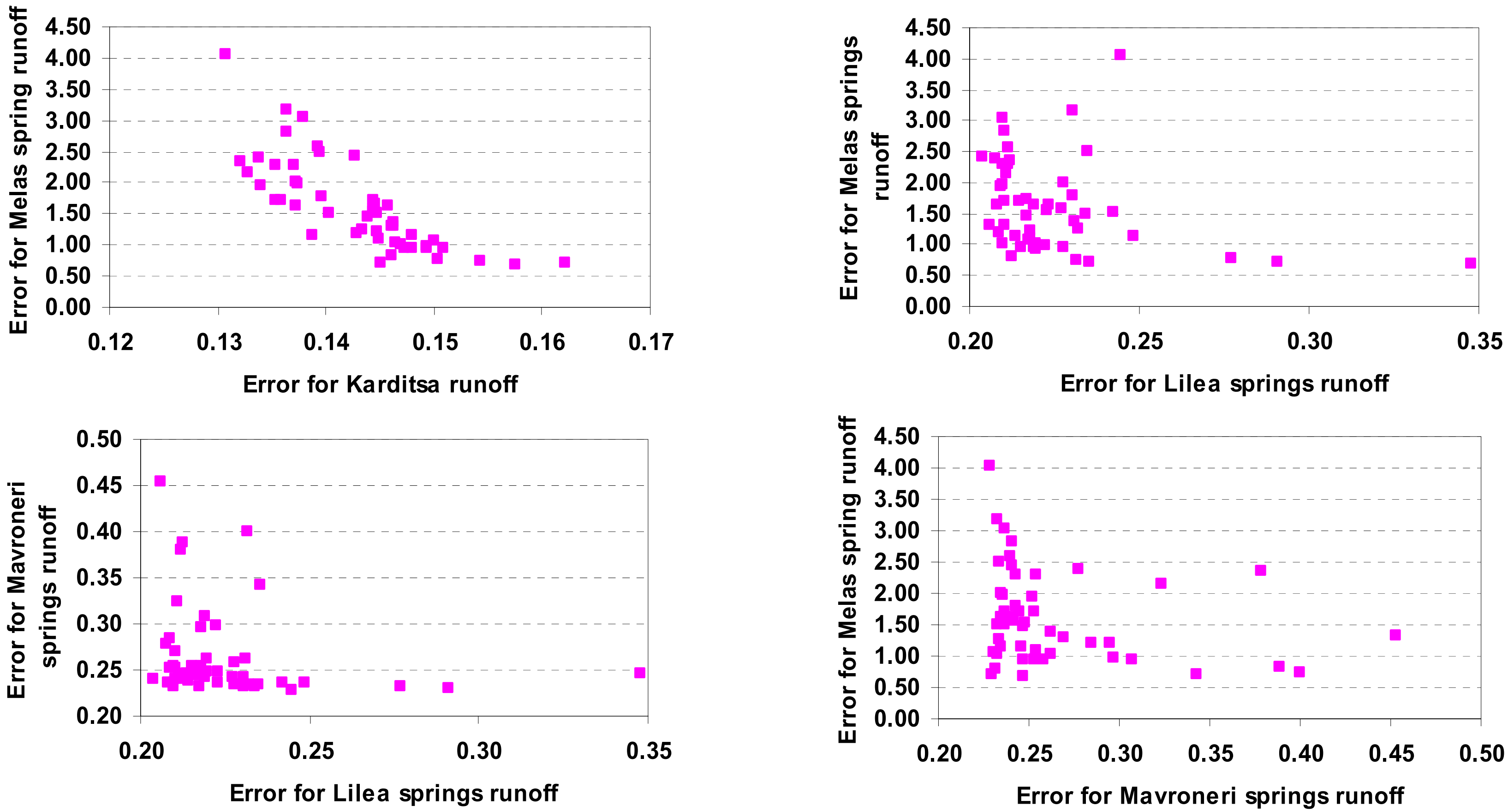




Multiobjective calibration of a complex hydrological model: Main assumptions

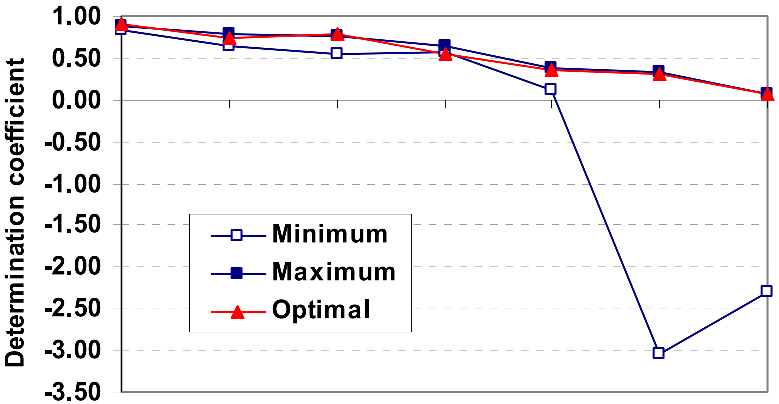
- **Observed series**: daily discharge measurements at the basin outlet (Karditsa tunnel), sparse (1-2 per month) discharge measurements at six main karstic springs, contributing more than 50% of total runoff
- **Control period**: October 1984-September 1990 (calibration period), October 1990-September 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) and recession rate for percolation (μ), assigned to each HRU, conductivity (C) 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

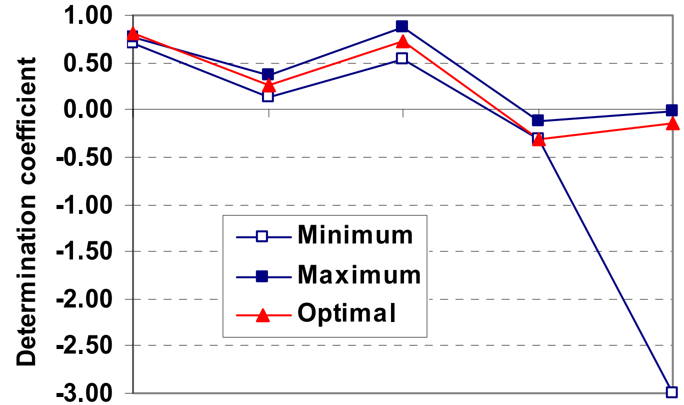


Trade-offs represent: (a) **modelling errors** due to the complexity of processes (negative correlation of some spring hydrographs with precipitation); and (b) **data errors**, due to the construction of control series based on few observations

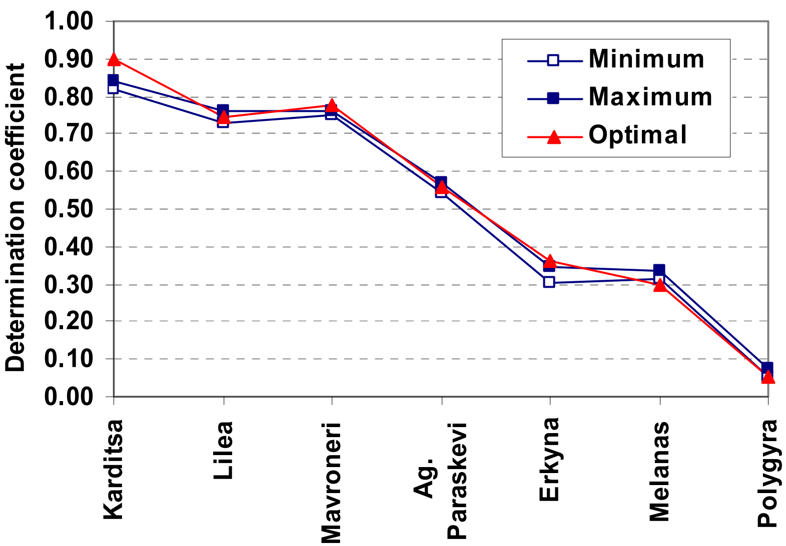
Multiobjective calibration of a complex hydrological model: Restricting the objective space



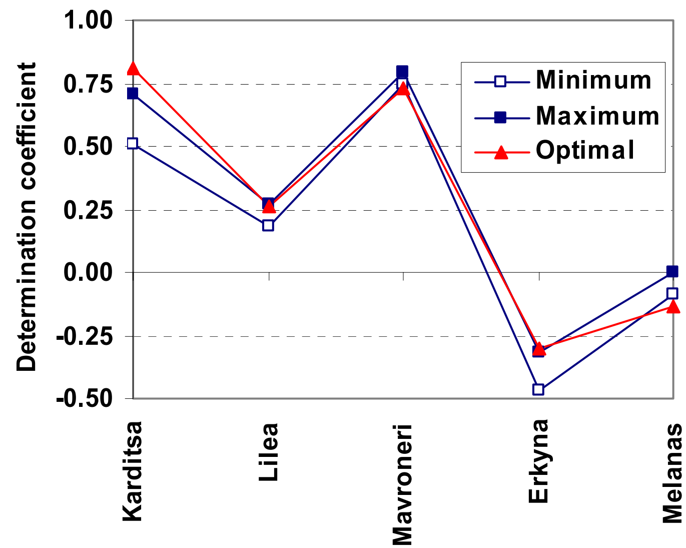
Unbounded objective space, calibration



Unbounded objective space, validation



Bounded objective space, calibration



Bounded objective space, validation

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.

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Poster presentation of the hydrological model:

Friday, 29 April 2005, 17:30 - 19:00, area Z028

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