Model Calibration and Uncertainty

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After this lecture you will

- be able to **describe** sources of uncertainty in hydrological models
- be able to **identify and classify** model parameter calibration procedures
- be able to **explain and discuss** different model performance measures
- be able to **analyze and assess** different model evaluation techniques

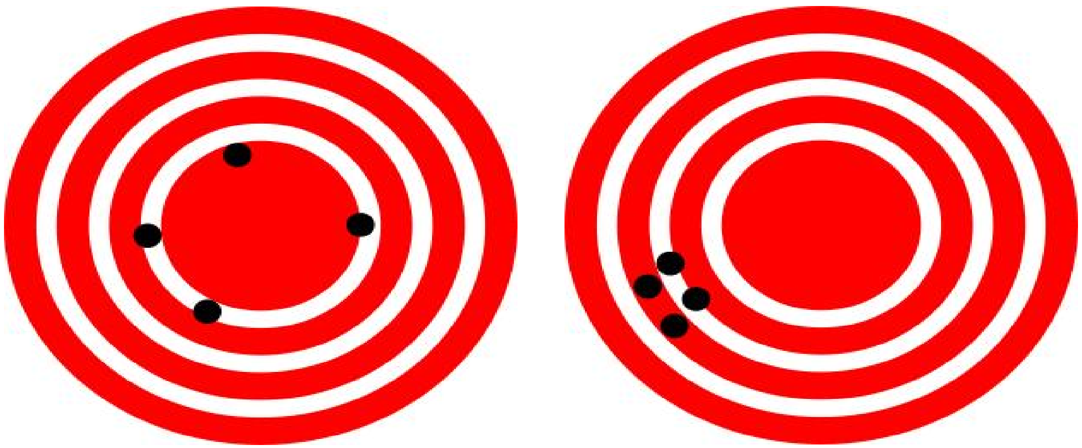
Hydrological models

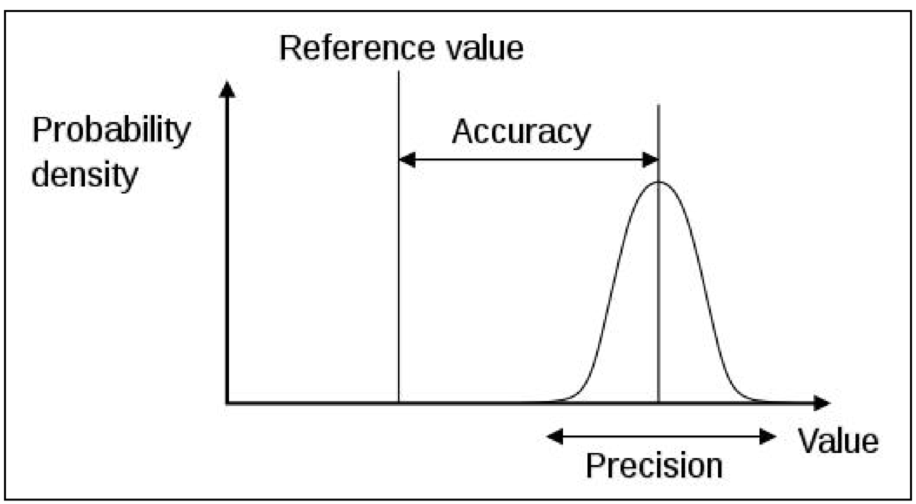
- $\boldsymbol{Q} \leftarrow m(\boldsymbol{X}, \vartheta, \boldsymbol{S_0})$
  - $\boldsymbol{Q}$: system response
  - $\boldsymbol{m}$: hydrological model
  - $\boldsymbol{X}$: inputs
  - ϑ: model parameters
  - $\boldsymbol{S_0}$: initial and boundary conditions
- Each component is subject to uncertainty

Sources of uncertainty

Low precision
High accuracy

High precision
Low accuracy





Sources of uncertainty

- **Observational uncertainty**

  (i) instrument **precision**

  (ii) measurement **accuracy**

  (iii) spatial and temporal **heterogeneity**

  (How representative is the measurement?)

  Present in:

  (i) input (e.g. rain, evaporation)

  (ii) response (runoff, groundwater, chemical composition)

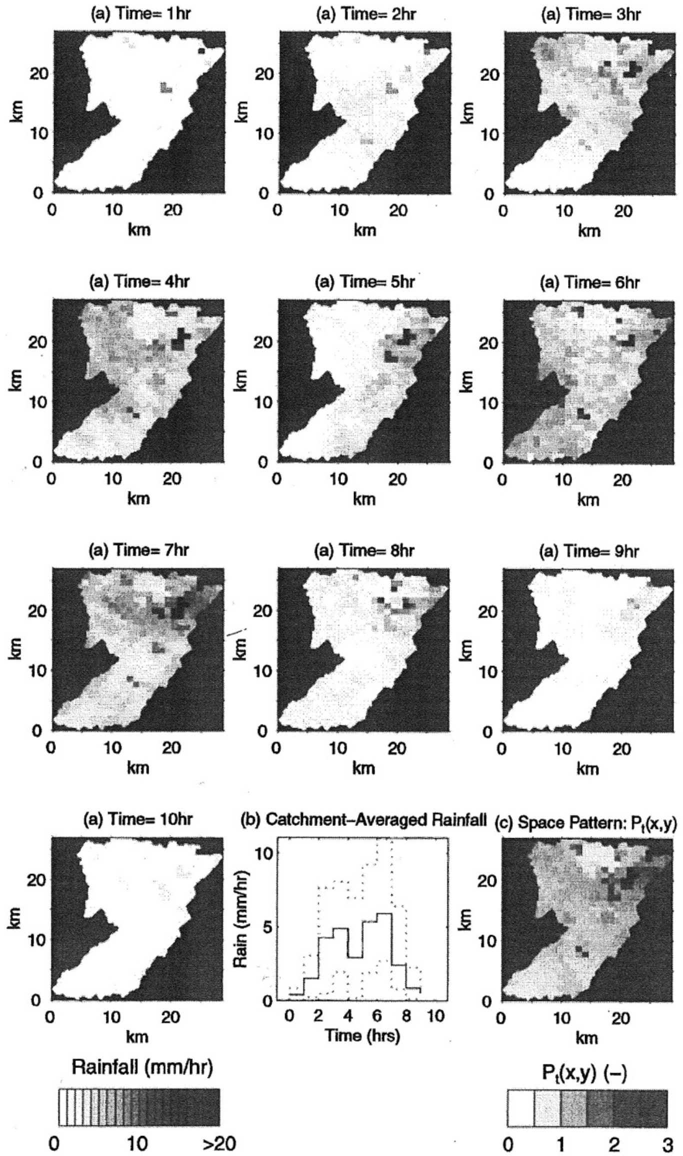
- **Model structure uncertainty**

  Imperfect conceptualization of system

- **Model parameter uncertainty**

  Different parameter combinations can yield same result

Sources of uncertainty



Sources of uncertainty

Example:

Catchment 5km^2,

6 rain gauges

Proportion of rain gauges that record rain when one of them is recording rain

Sources of uncertainty

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Catchment 5km^2,

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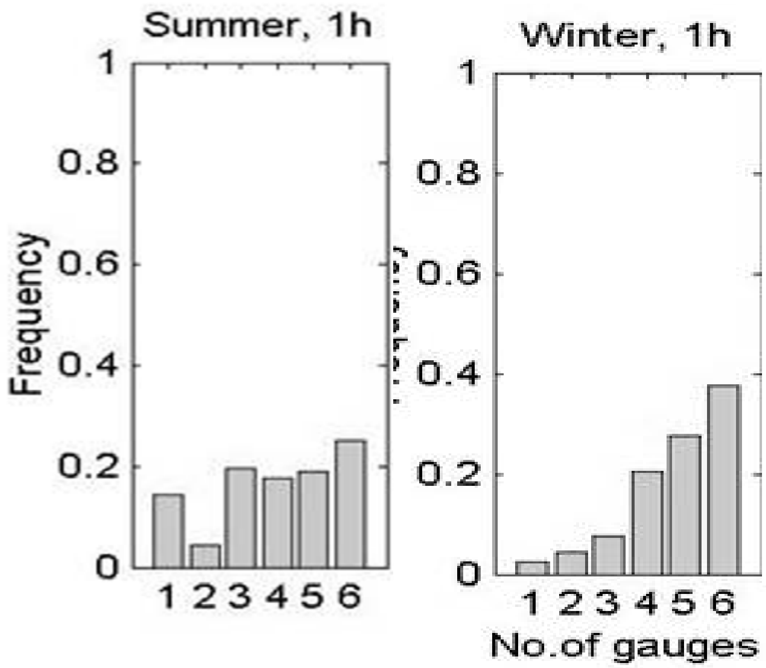

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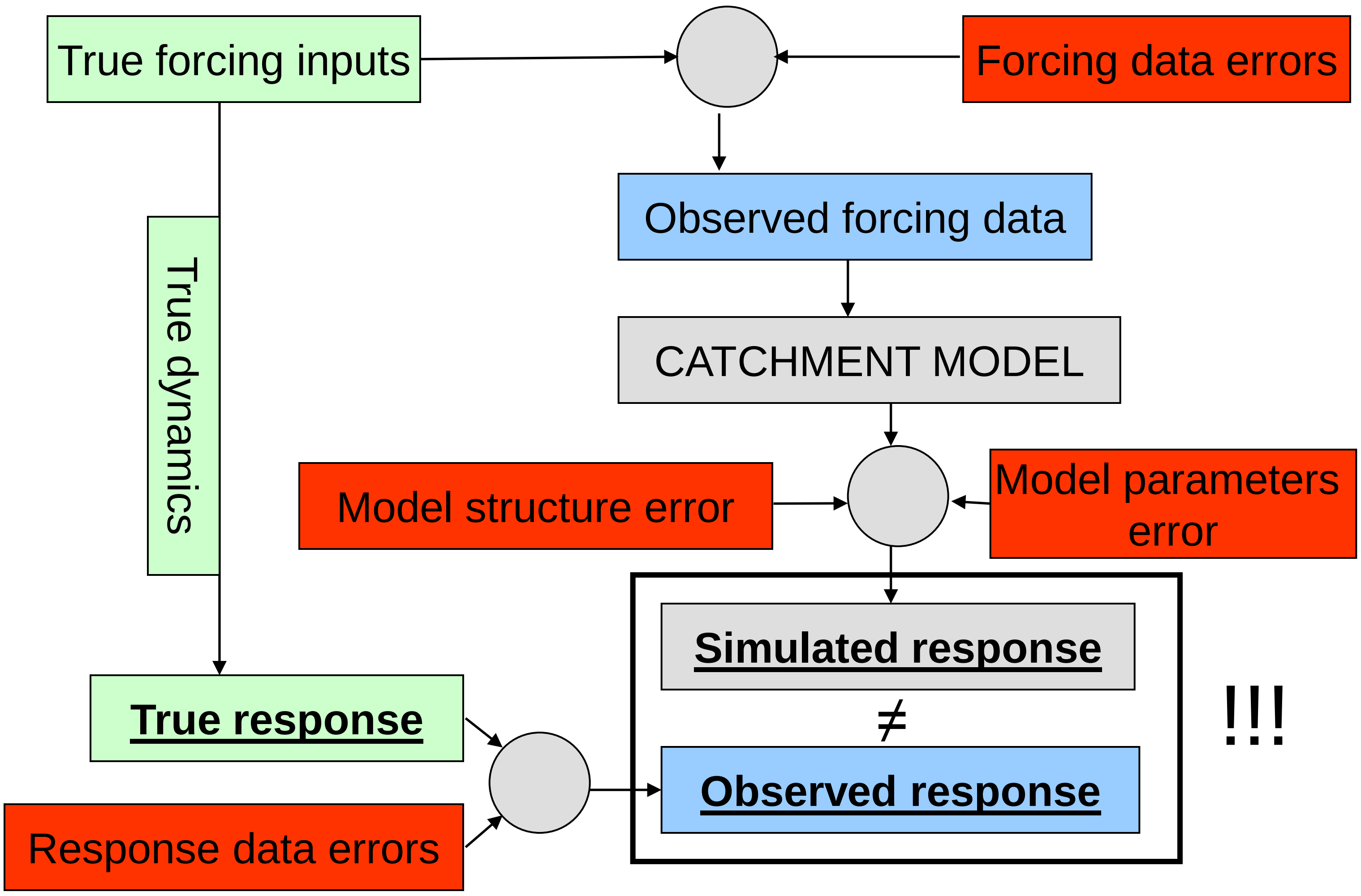
Error propagation in catchment modelling



Parameter estimation

$\boldsymbol{Q} \leftarrow m(\boldsymbol{X}, \vartheta, \boldsymbol{S_0})$

- Direct measurement (*problem of scale)*
- Derivation from analysis of measured variables (*problem of scale, uniqueness of place)*
- Calibration

Calibration

- Calibration is a **process of parameter adjustment** (automatic or manual), until observed and calculated output time-series show a sufficiently high degree of similarity

- Model parameters are conceptual representations of abstract watershed characteristics - **not independently measurable**

Manual calibration

- Also called “Trial-and-error”
- Based on:

  a) Visual inspection of the hydrograph

  b) Different measures of performance
- Can produce good results but:

  a) time consuming

  b) not objective

Automatic calibration

- Computer based
- Fast
- Objective

but

- The resulting hydrographs are often perceived to be inferior to those produced through manual calibration from the hydrologist's point of view

Automatic calibration

- Parameter calibration problem is set as an optimization problem
- Optimization means finding the parameters that maximise or minimise a certain function
- Model performance is expressed as a function of model parameters (objective function N)

$$\boldsymbol{Q_m} = m(\boldsymbol{X}, \vartheta, \boldsymbol{S_0})$$

$\boldsymbol{Q_o}$: *observed system response*

$$N_{obj} = f(\boldsymbol{Q_m}, \boldsymbol{Q_o})$$

Objective functions

- Objective functions aggregate model residuals in time

- Different functions can express the error associated to different aspects of the simulation (e.g. high flow, low flow, bias, groundwater dynamics)

Objective functions

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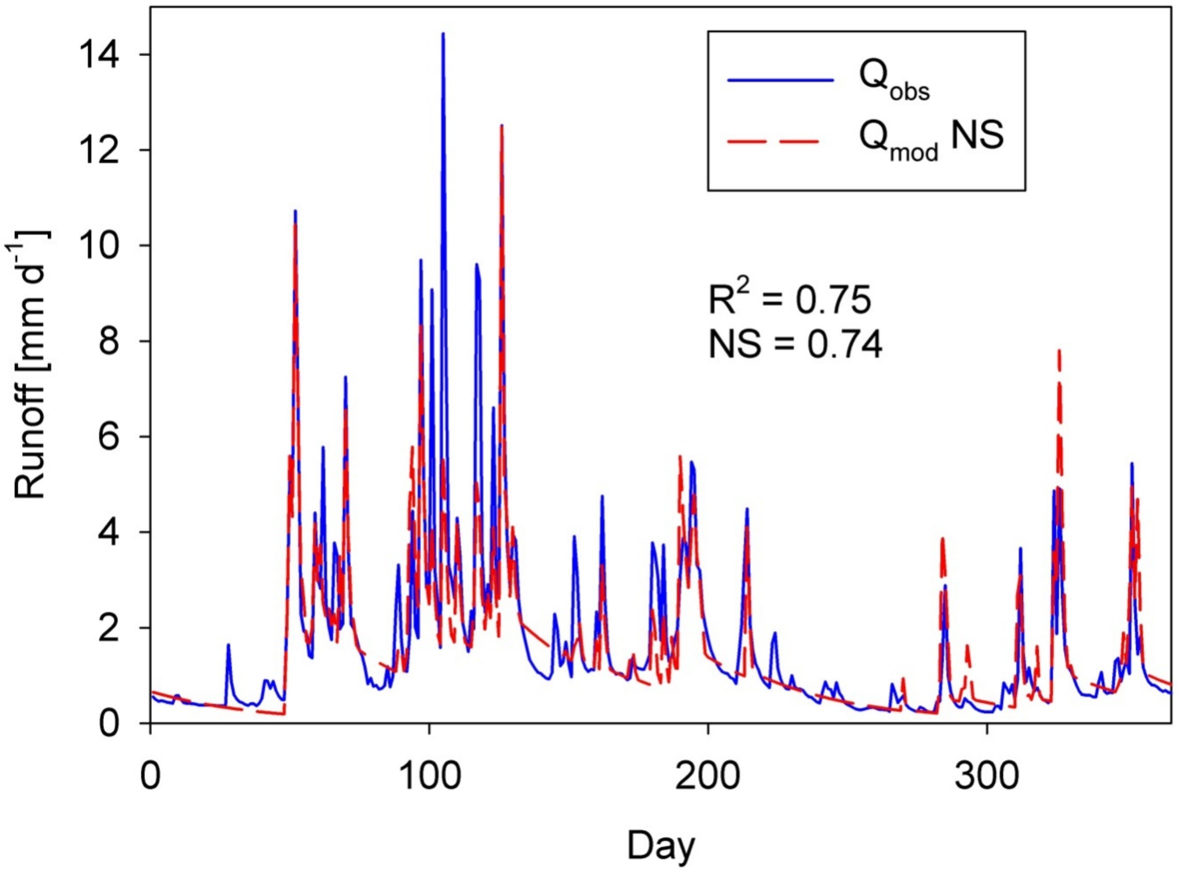


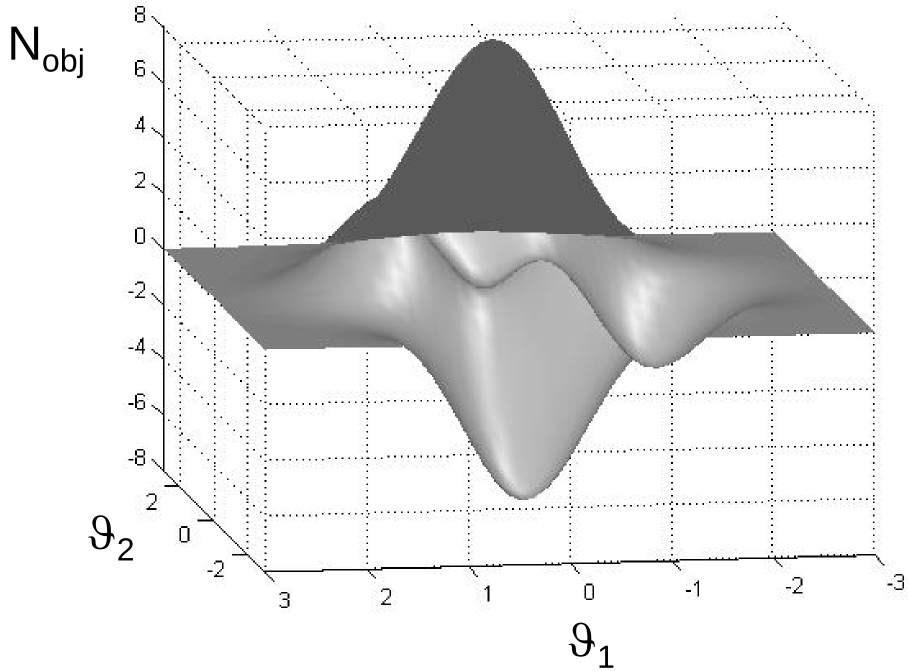
- Bias (0 ≤ Bias ≤ ∞)

$$N_{Bias} = \sum_{i=1}^{n}\left(Q_{s,i} - Q_{o,i}\right)$$

Optimization of objective functions

How does the **response surface** of objective function ***N_{obj}=f(ϑ)*** look like?

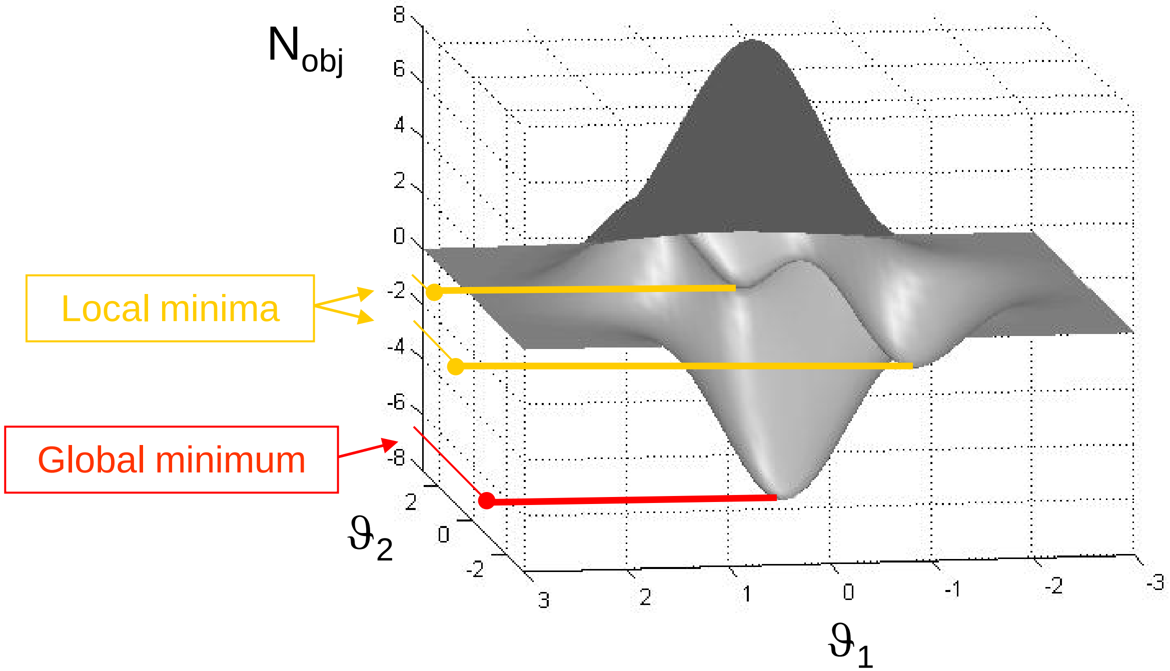
- **Complex** landscapes with multiple curving ridges
- Small- and large-scale **discontinuities**
- **Multiple optima**



Optimization of objective functions

Search strategies for finding optimal parameter set

- Local search strategies can converge in a **local minimum** instead of the global one
- Solved with **global search strategies** that use randomized search



Optimization of objective functions

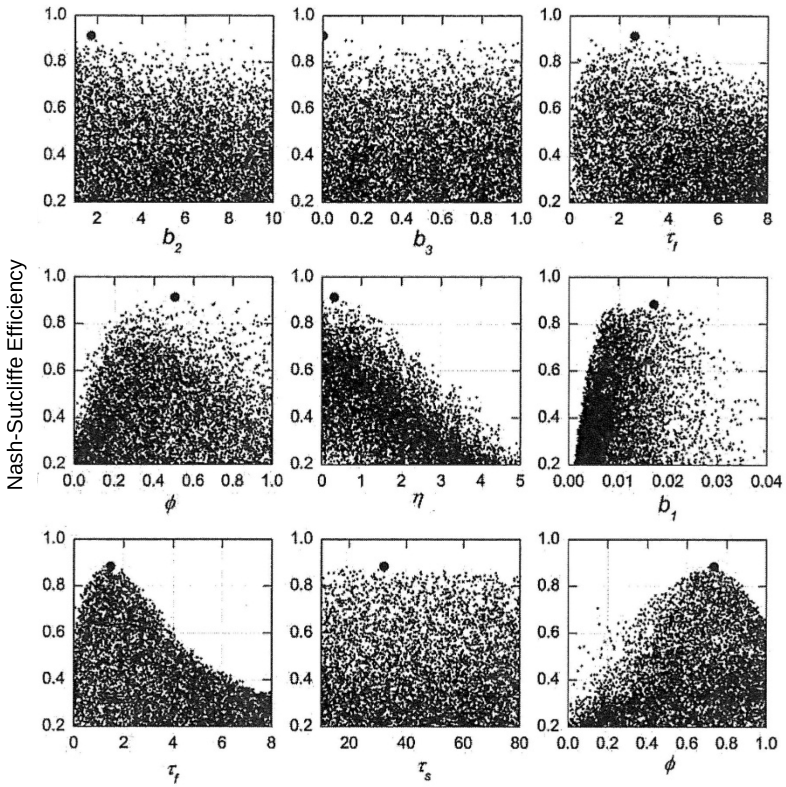
Global search strategies for finding optimal parameter set:

- **Stochastic**
  - (a) Monte-Carlo sampling,
  - (b) Simulated annealing,…
- **Heuristic**
  - (a) Genetic algorithms,
  - (b) Shuffled Complex Evolution,
  - (c) Ant-Colony and Particle Swarm methods,…

Optimization of objective functions

Monte Carlo Sampling

- Randomly sample each parameter from prior distribution
- Very simple
- Time consuming
- Although good information about the region of optimal parameters, **best** parameters unlikely to be found

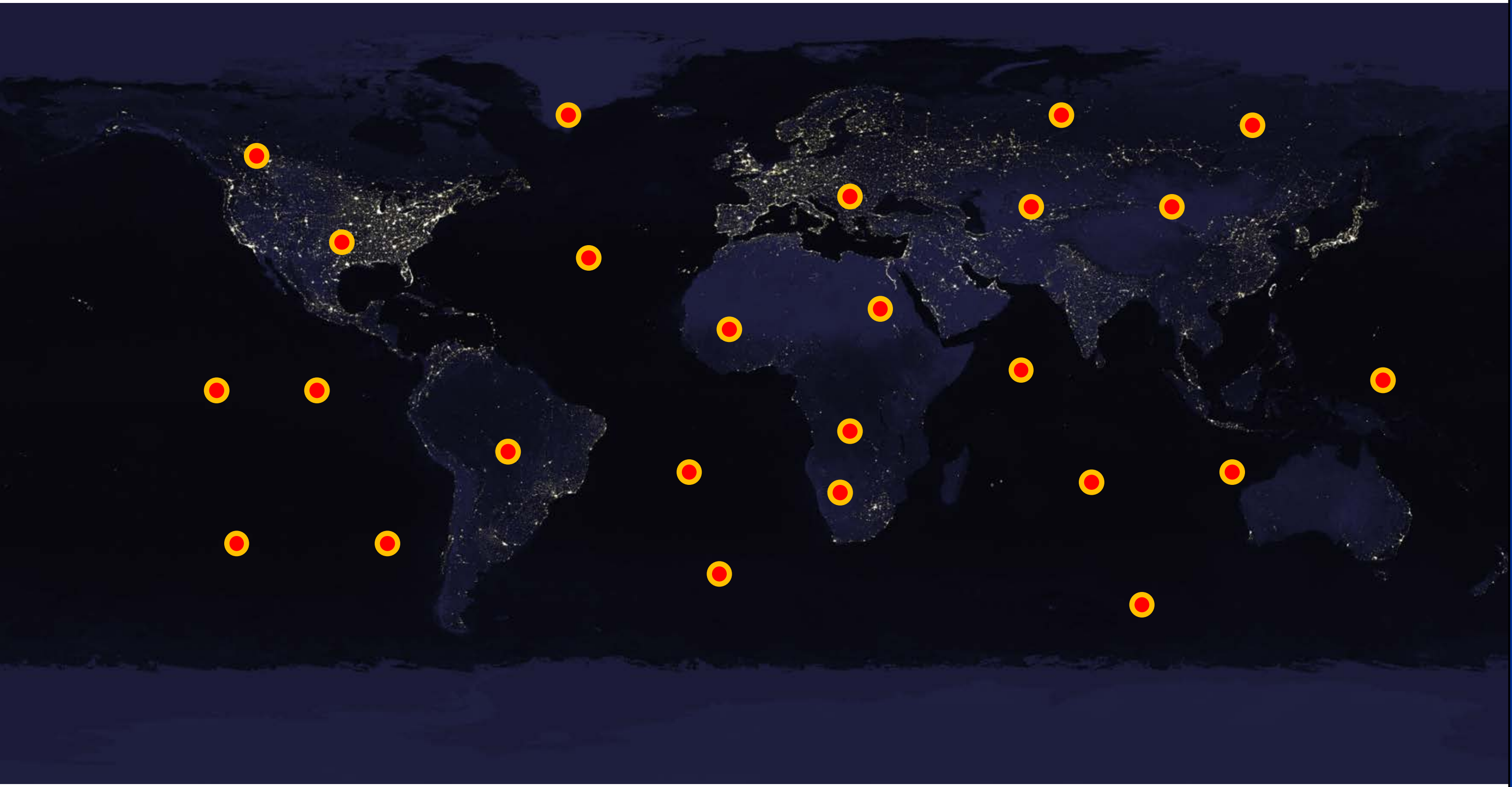


Optimization of objective functions

Evolutionary algorithms

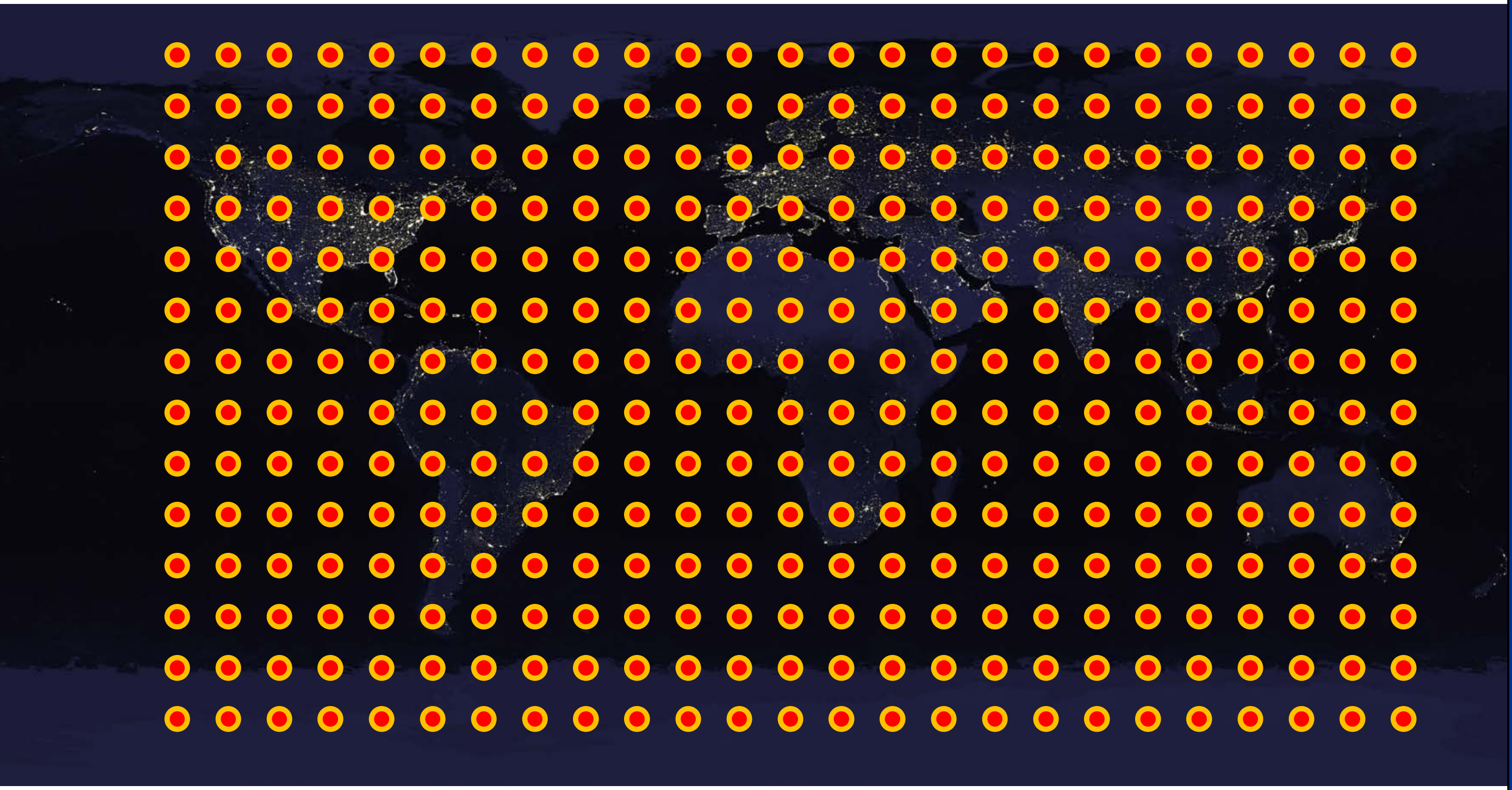
Optimization of objective functions

Evolutionary algorithms



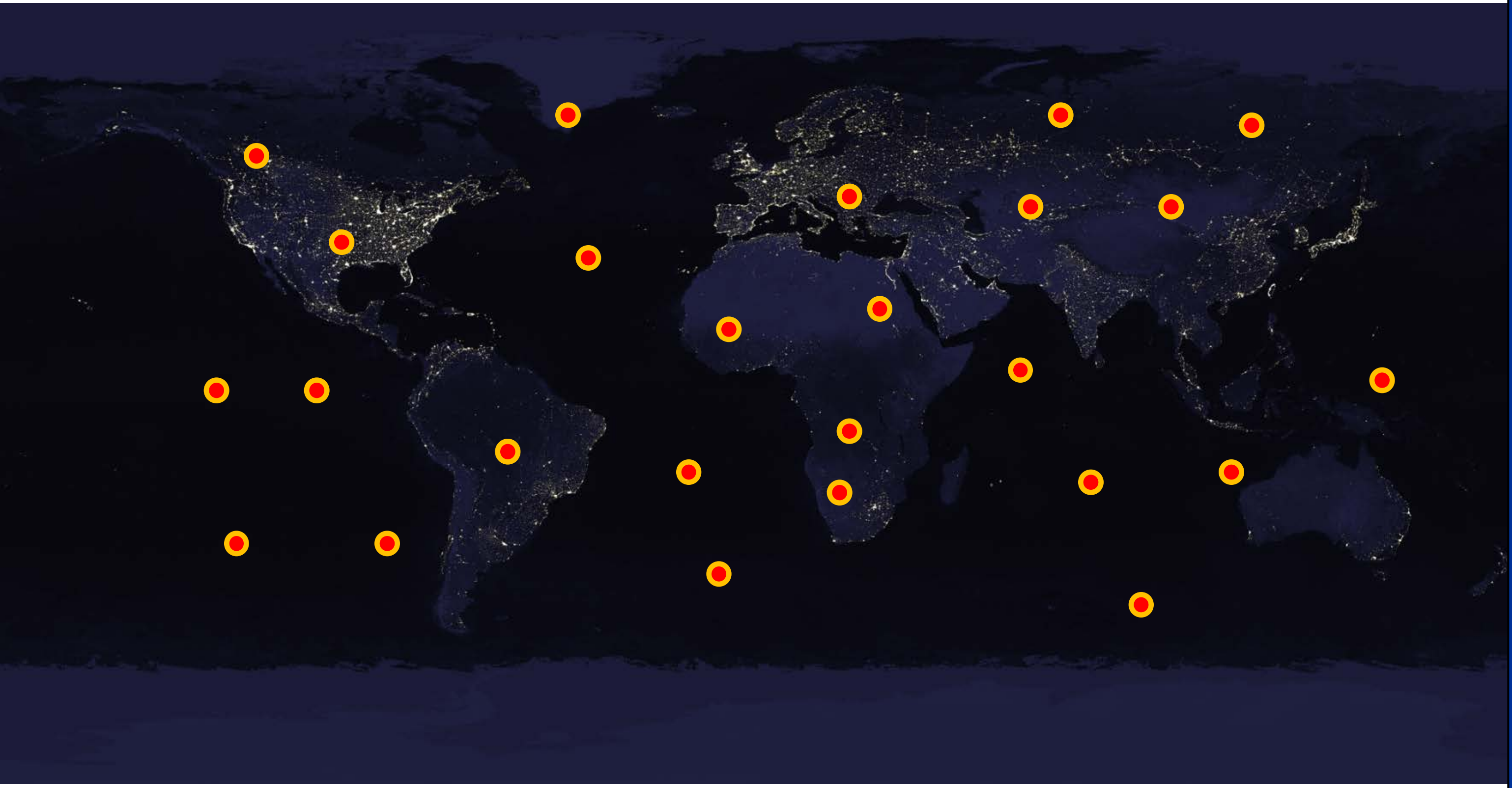
Optimization of objective functions

Evolutionary algorithms



Optimization of objective functions

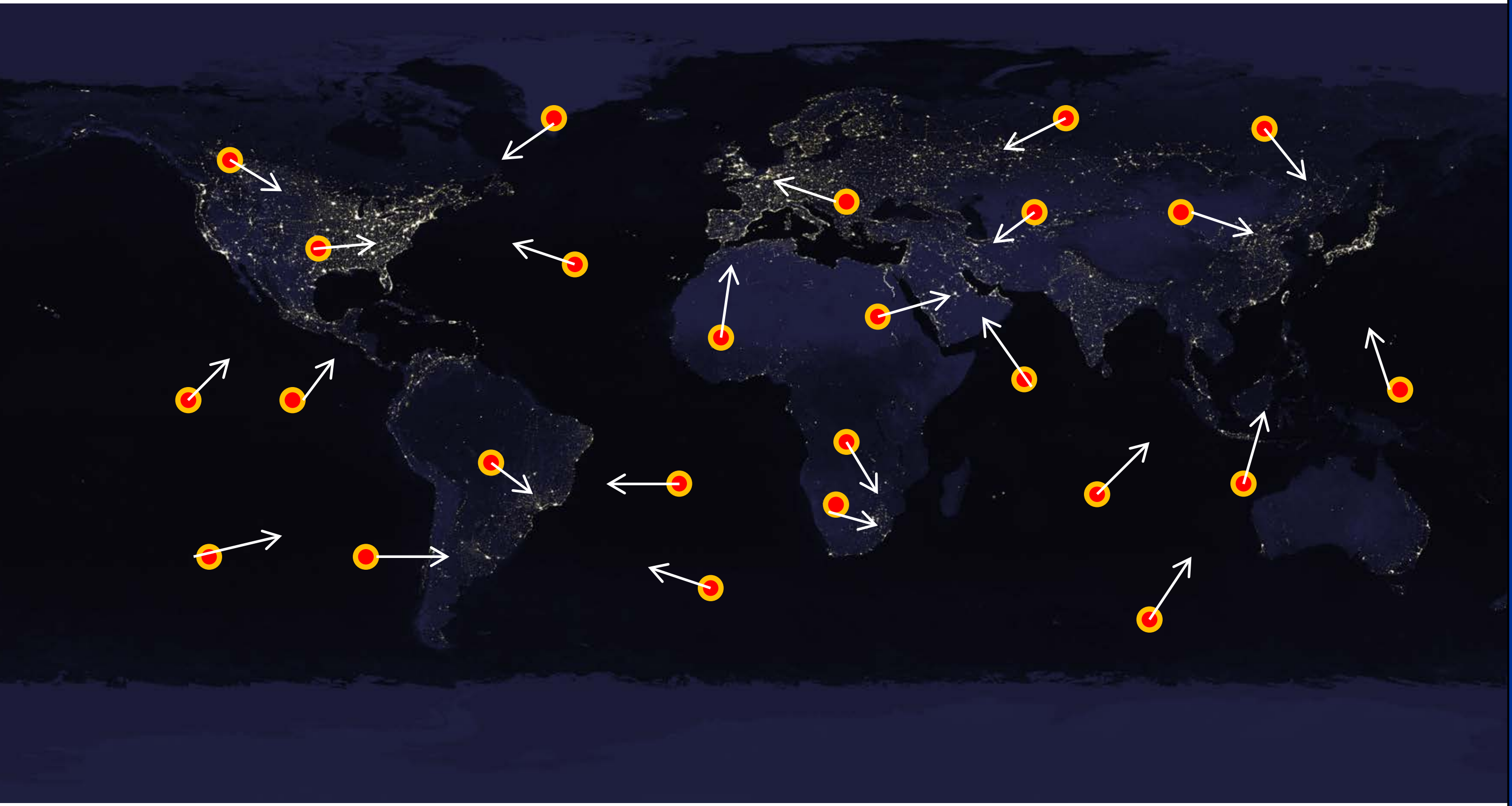
Evolutionary algorithms



- ✓ Objectives
- ✓ Sources of uncertainty
- ✓ Why do we care?
- ✓ Calibration
- ✓ Objective functions
- **Optimization**
- Parameter uncertainty
- New approaches
- What have we learned?

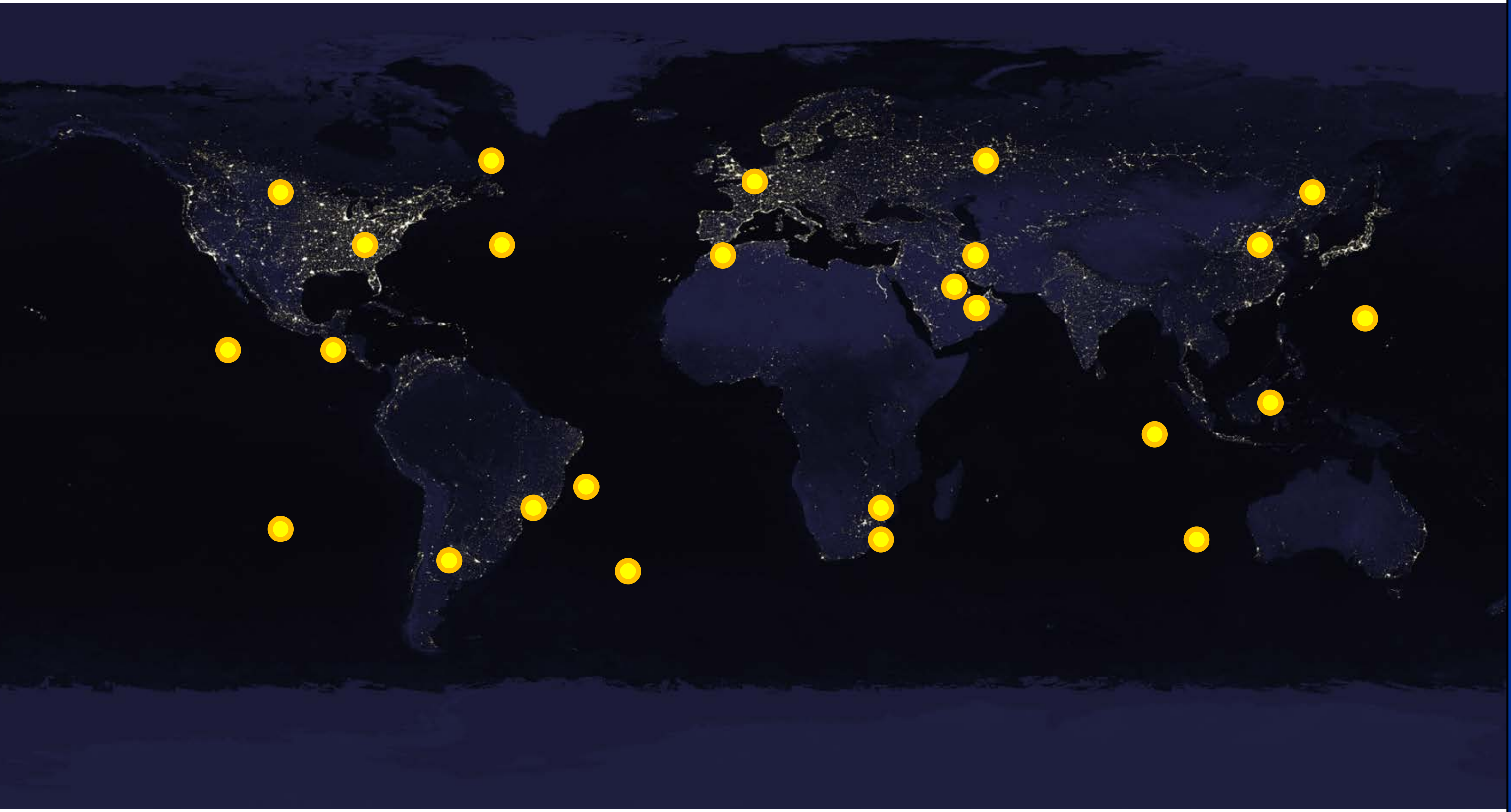
Optimization of objective functions

Evolutionary algorithms



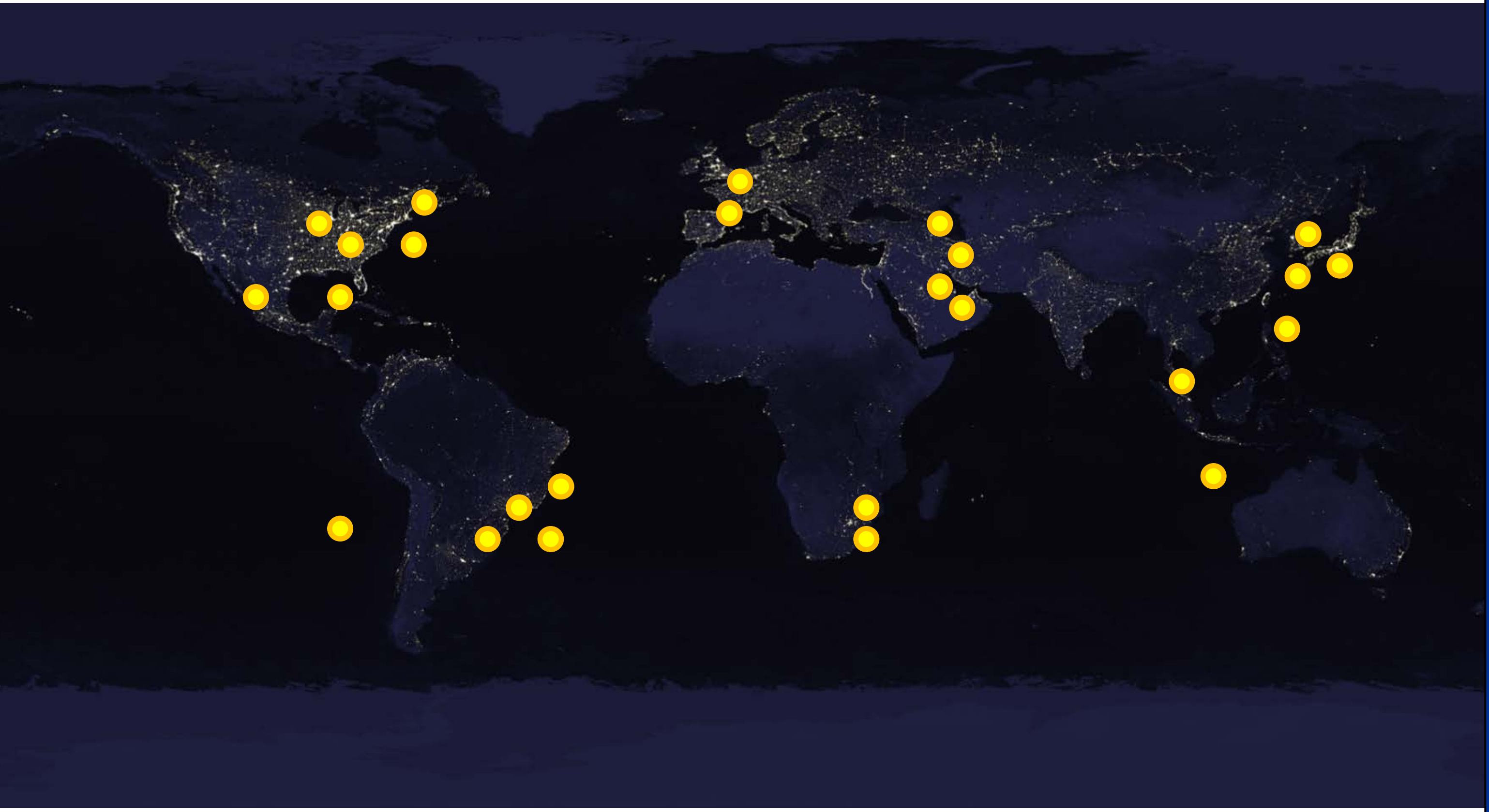
Optimization of objective functions

Evolutionary algorithms



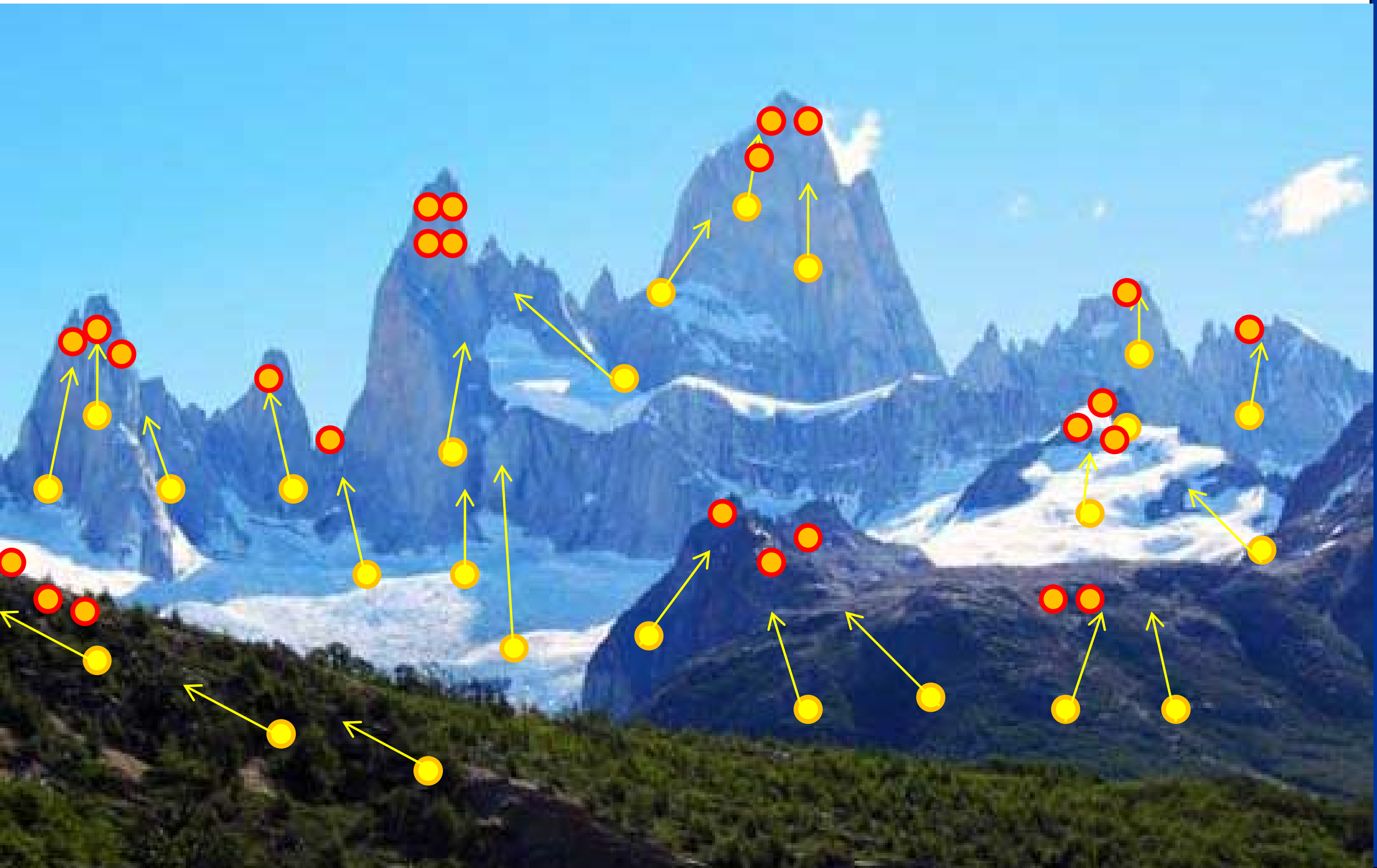
Optimization of objective functions

Evolutionary algorithms



Optimization of objective functions

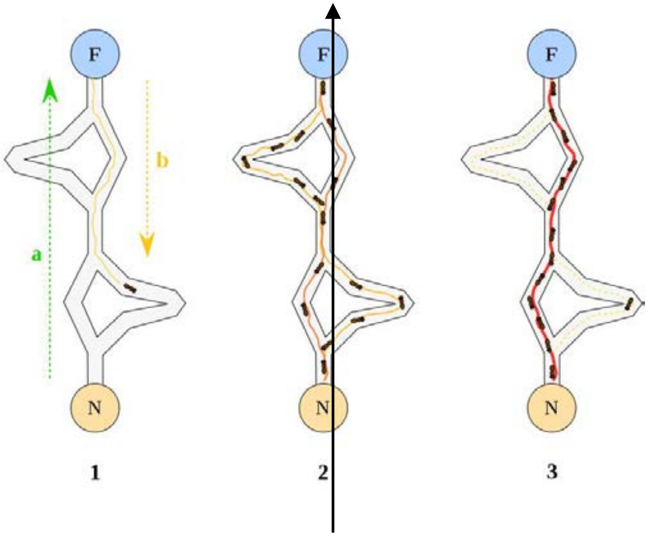
Evolutionary algorithms



Optimization of objective functions

<u>Ant-Colony optimization</u>

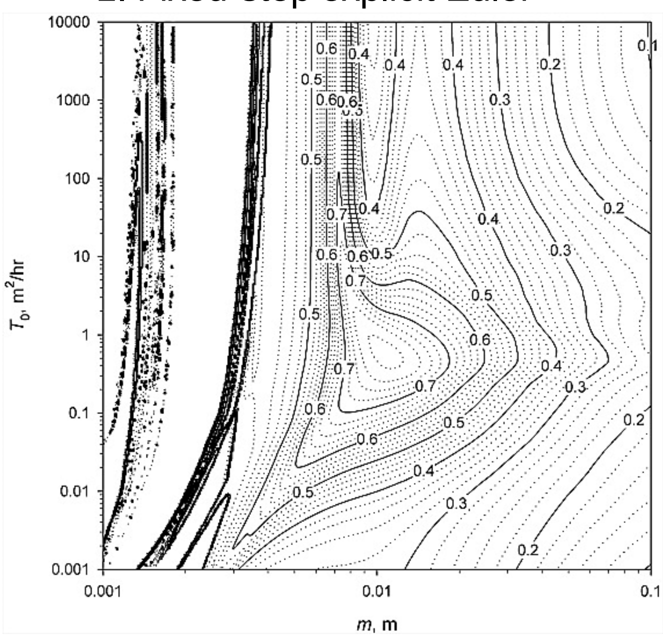
- Mimics self-organizing dynamics of nature
- Based on **collective "intelligence"** of insects
- Collective of ants finds **shortest route** to food
- Leave pheromone trail, attracting other ants
- The more ants, the more pheromone, the more ants → **positive feedback process** (self-organization)



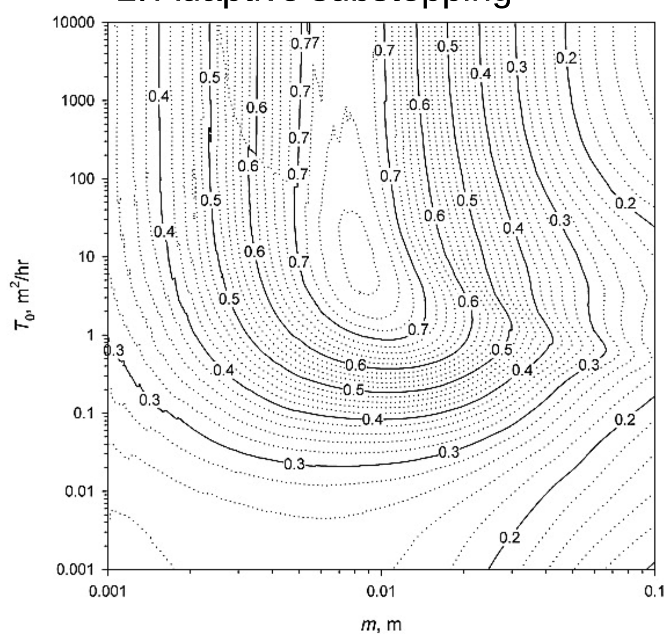
Optimization of objective functions

- Complex shape of objective functions can be a numerical artifact
- Remember exercise 1
- Using a too large time step introduces large numerical error
- This can affect the shape of the objective function

1. Fixed-step explicit Euler



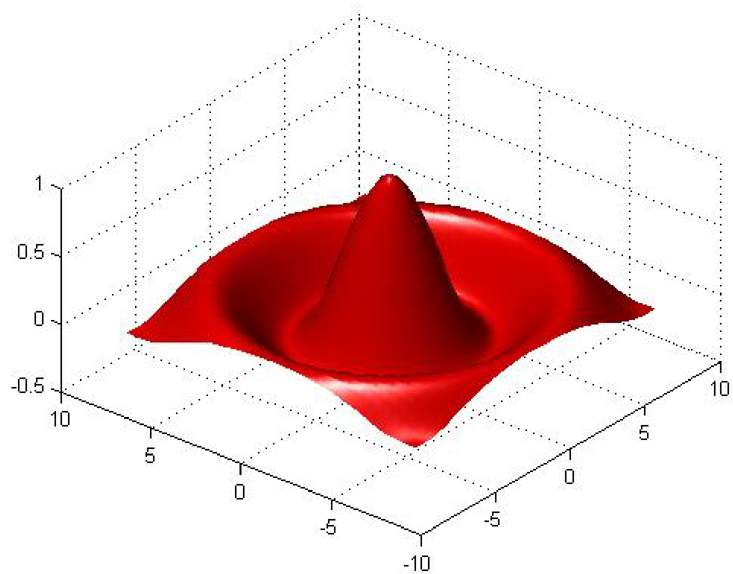
2. Adaptive substepping



Optimization of objective functions

Multiple optima

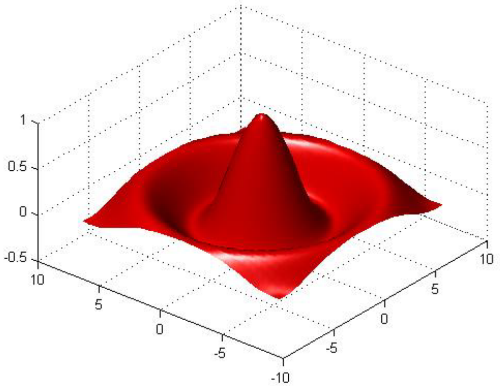
- Response surface can have more than one optimum
- Many parameter sets may yield equally good results
- This has impact on parameter and predictive uncertainty



Parameter uncertainty

Multiple optima – different approaches

- Accept existence of multiple optima and introduce concept of **equifinality** (GLUE)
- Use of Bayesian statistics to address in a **formal way** problems related to data uncertainty
- Accept that a single objective function is not appropriate: instead use **more criteria and objectives** to constrain the problem (Multi-criteria, multi-objective calibration)



Parameter uncertainty

GLUE

(Generalized Likelihood Uncertainty Estimation)

- "The concept of a **single description of reality** may remain a philosophical axiom or theoretical aim but is **impossible** to achieve in practice"

- "So we must accept that there may be **many feasible descriptions**, or a concept of **equifinality**, as the basis for a new approach"

(Keith Beven)

Parameter uncertainty

GLUE

(Generalized Likelihood Uncertainty Estimation)

- Rejects the concept of an optimum model and parameter set
- The existence of multiple likely models and parameter sets has been called **equifinality**

Parameter uncertainty

GLUE

(Generalized Likelihood Uncertainty Estimation)

(1) Prior to input of data into a model, all model structures and parameter sets have an **equal likelihood** of being acceptable

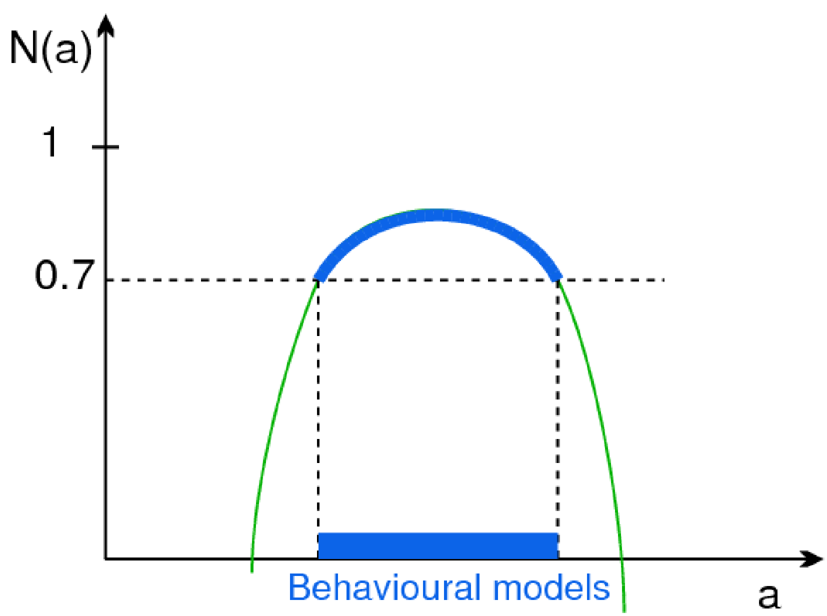
(2) A high number of parameter sets is generated via uniform Monte Carlo **sampling**

(3) The performance of each trial is assessed through a **likelihood measure** (e.g. Nash-Sutcliffe Efficiency)

Parameter uncertainty

GLUE

(4) Only models, i.e. parameter sets and model structures, whose likelihood measure is above a threshold are retained (**“behavioural models**”), all others are discarded (**“non-behavioural models”**)



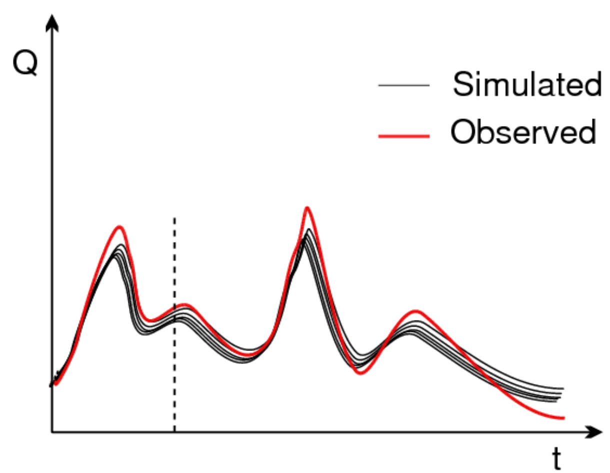
Parameter uncertainty

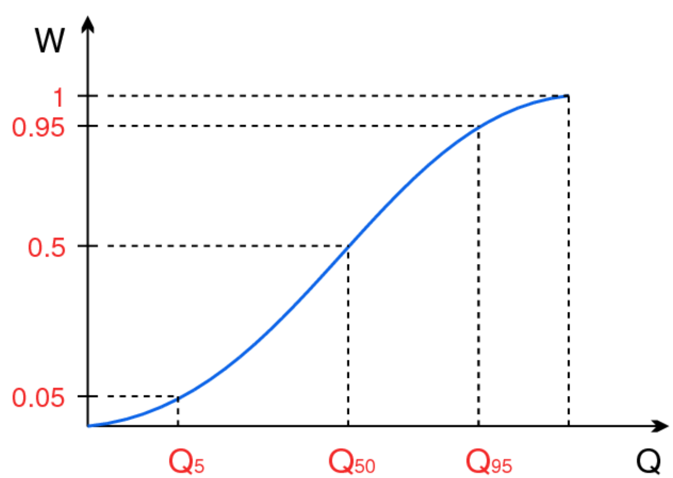
GLUE

(5) The calculated likelihoods are rescaled to a cumulative sum of 1

(6) For each time step, a cumulative distribution of simulated discharges is constructed using the rescaled weights

(7) Uncertainty bounds and median from cumulative distribution

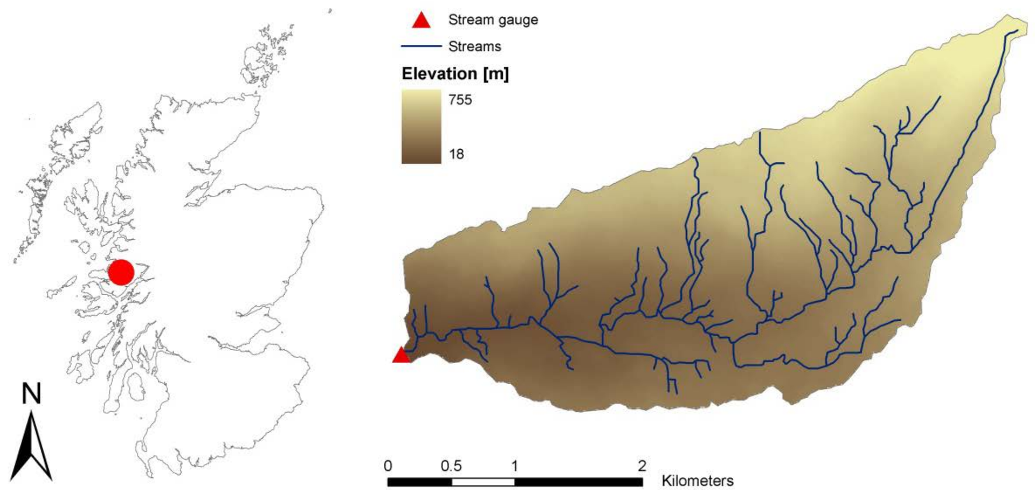




Parameter uncertainty

GLUE – example

- 10 km² catchment in Scotland
- Modelling tracer dynamics in stream
- 2 parameter model (α,β)



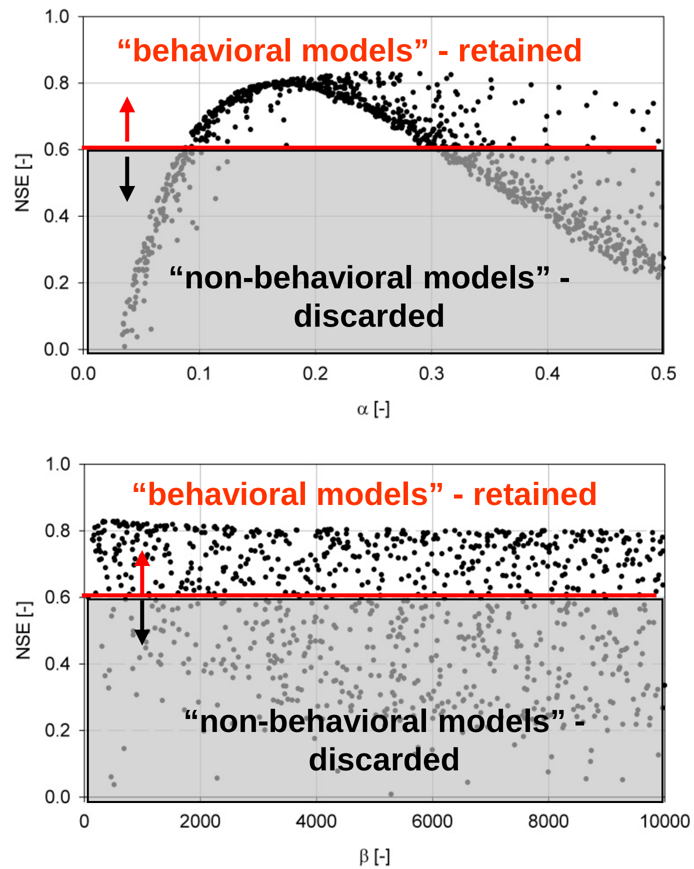
Parameter uncertainty

GLUE – example

- Likelihood measure: Nash-Sutcliffe efficiency (NSE)

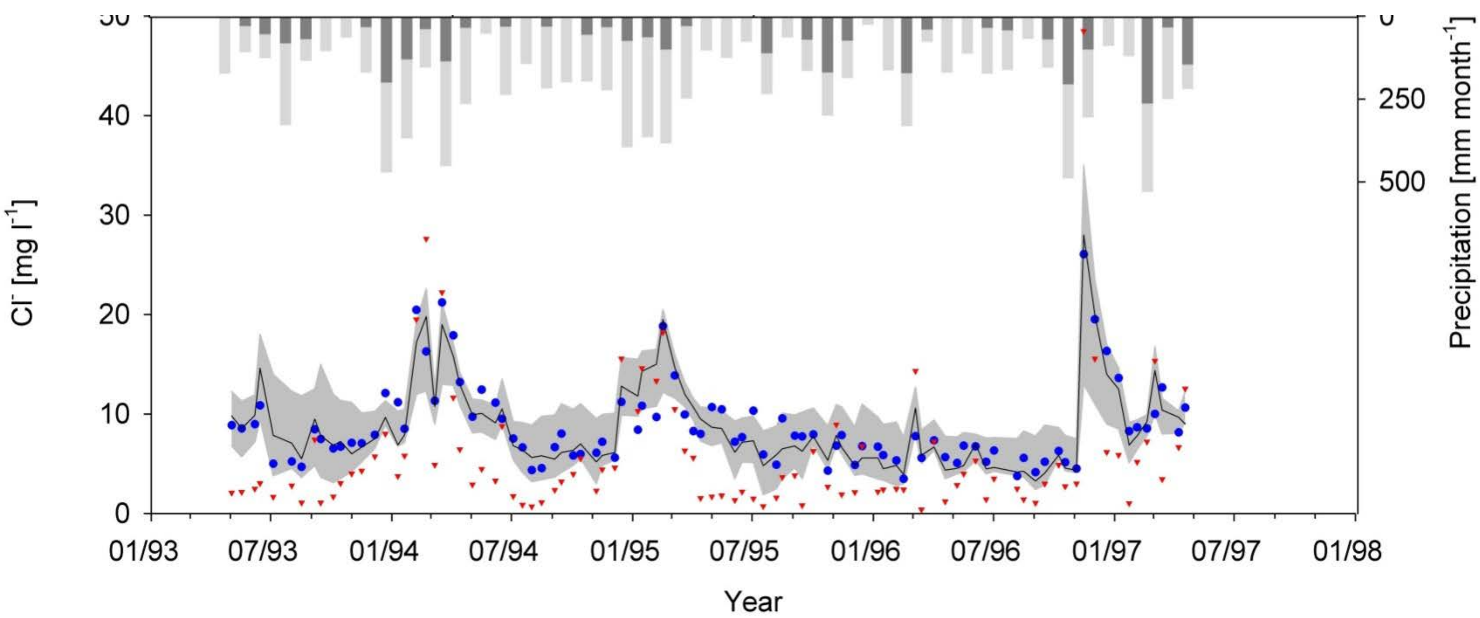
$$N_{NS} = 1 - \frac{\sum_{i=1}^{n} \left(Q_{s,i} - Q_{o,i} \right)^2}{\sum_{i=1}^{n} \left(Q_{o,i} - \overline{Q}_{o,i} \right)^2}$$

- Threshold of acceptance: $N_{NS} > 0.6$



Parameter uncertainty

GLUE – example



- ✓ Objectives
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- ✓ Optimization
- **Parameter uncertainty**
- New approaches
- What have we learned?

Parameter uncertainty

GLUE

- Glue introduces the problem of equifinality in hydrological modelling
- Easy to understand and implement
- Allows model evaluation with respect to performance and uncertainty
- **Limitation:** subjectivity (choice of threshold!)
- To limit subjectivity:

  (a) "Limits of acceptability" approach

  (b) Adjust threshold so that x% of observations fall within uncertainty interval

  (c) Accept all models, but give higher weight to better models, e.g. NSE^p

Parameter uncertainty

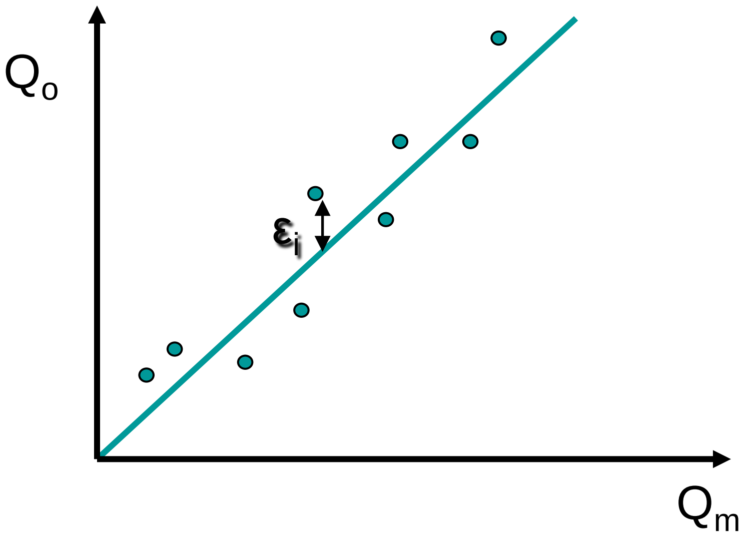
Formal Bayesian approach

- Likelihood functions should be based on hypotheses of the error
- Example:

$Q_{o,i} = Q_{m,i} + \varepsilon_i$

$\varepsilon_i \sim N(\mu=0; \sigma^2)$

$$P(Q_{o,i} / \vartheta) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(Q_{o,i} - m_i(\theta))^2}{2\sigma^2}}$$



Parameter uncertainty

Formal Bayesian approach

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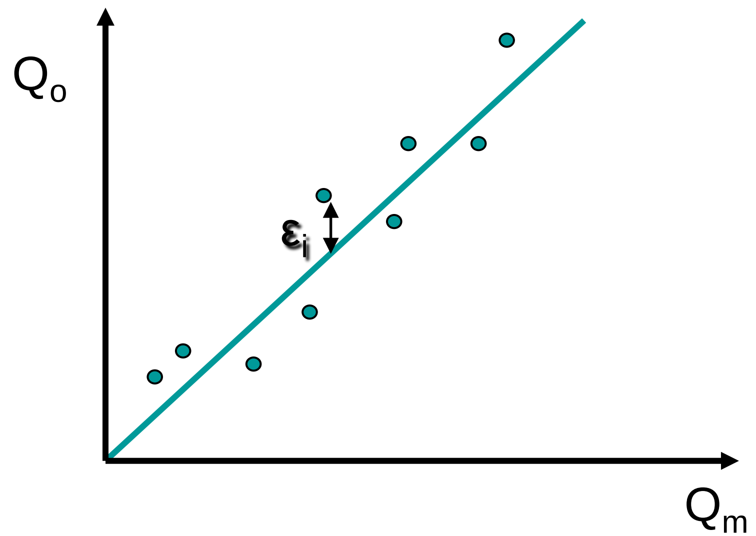


$$P(Q_{o,i} / \vartheta) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(Q_{o,i} - m_i(\theta))^2}{2\sigma^2}}$$

$$P(Q_o / \vartheta) = \left(\sigma\sqrt{2\pi}\right)^{-n} \prod_{i=1}^{n} e^{-\frac{(Q_{o,i} - m_i(\theta))^2}{2\sigma^2}} = \left(\sigma\sqrt{2\pi}\right)^{-n} e^{-\sum_{i=1}^{n}\frac{(Q_{o,i} - m_i(\theta))^2}{2\sigma^2}}$$

$$P\left(\vartheta / Q_o\right) = \frac{P\left(Q_o / \vartheta\right) P\left(\vartheta\right)}{P\left(Q_o\right)}$$

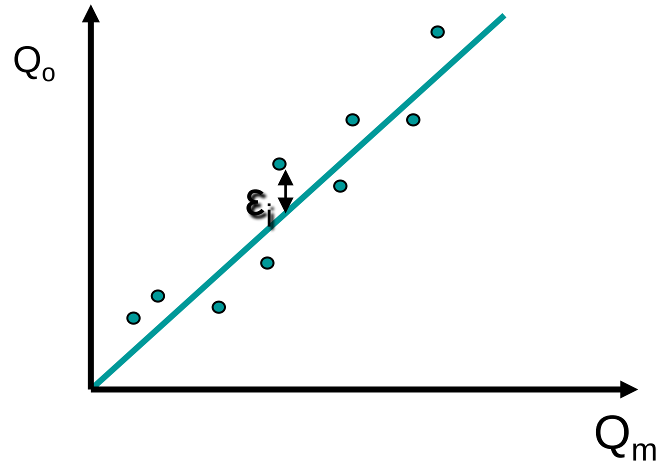
Parameter uncertainty

Formal Bayesian approach

For Bayesian statistics estimating θ using least squares means adopting several **assumptions**:

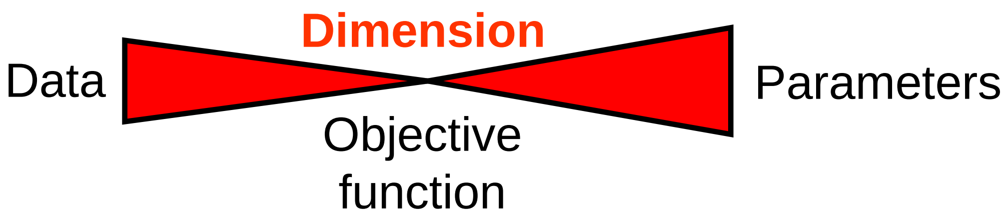
(a) model is correct

(b) error is normally distributed, uncorrelated, with constant variance (homoscedastic) and zero mean



Parameter uncertainty

Multi-objective calibration



- Data contain different signatures of catchment behaviour
- Information contained in the data represented by a single number
- Information represented by this number is then transferred to the model parameters
- Ideally parameter dimension should be the same as objective function dimension

Parameter uncertainty

Multi-objective calibration

Acceptable parameter range can be constrained by defining multiple optimization targets:

(a) **Multiple objective functions** (objectives), e.g. NS, NS_{log}, R^2, to evaluate one single modelled time-series, e.g. streamflow

(b) Objective functions to evaluate **multiple modelled variables** (criteria), e.g. stream flow, groundwater, chemical composition

(c) Objective functions in the **frequency domain**, e.g. fit flow duration curves or frequency spectrum

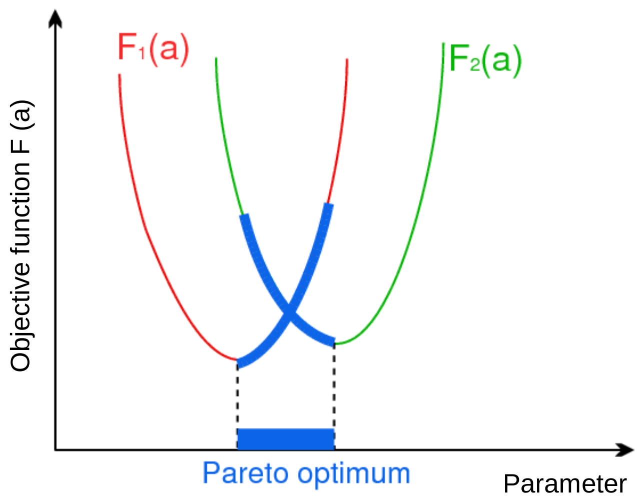
(c) Combinations of (a), (b) and (c)

Parameter uncertainty

Multi-objective calibration

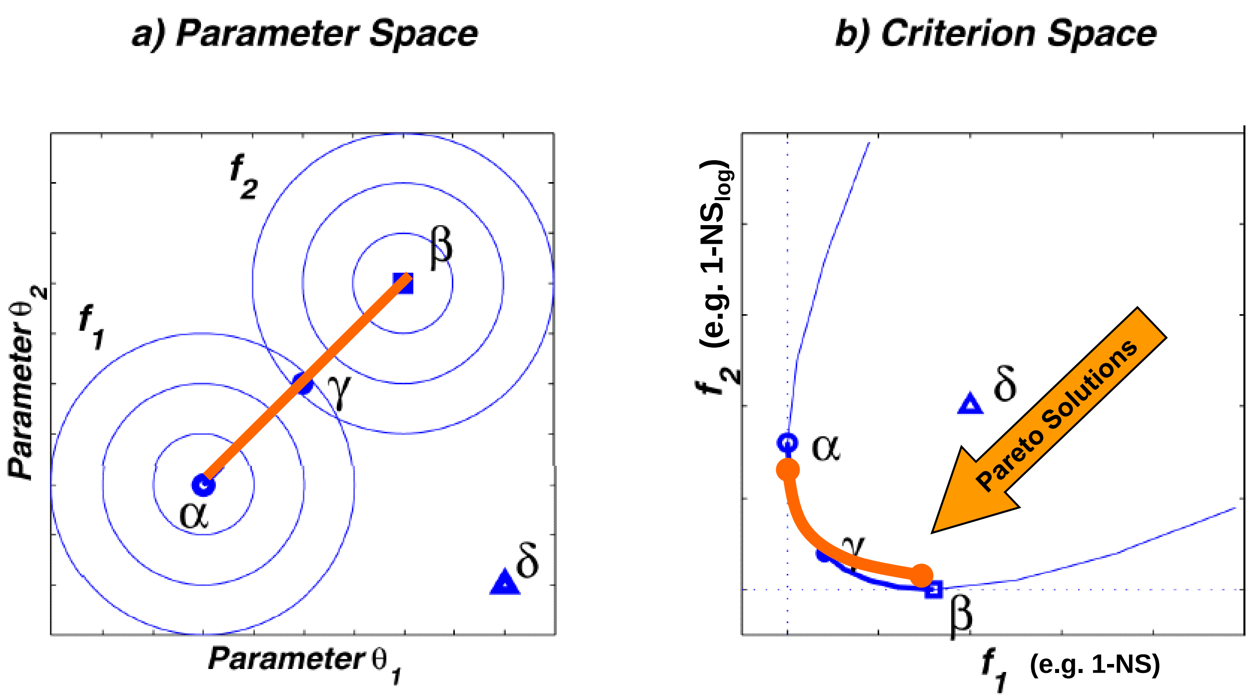
Pareto Optimality

- Not possible to find two points within the Pareto set such that one has a better performance than the other with respect to all objective functions
- For all non-members there exists at least one member that has a better performance with respect to all objective functions



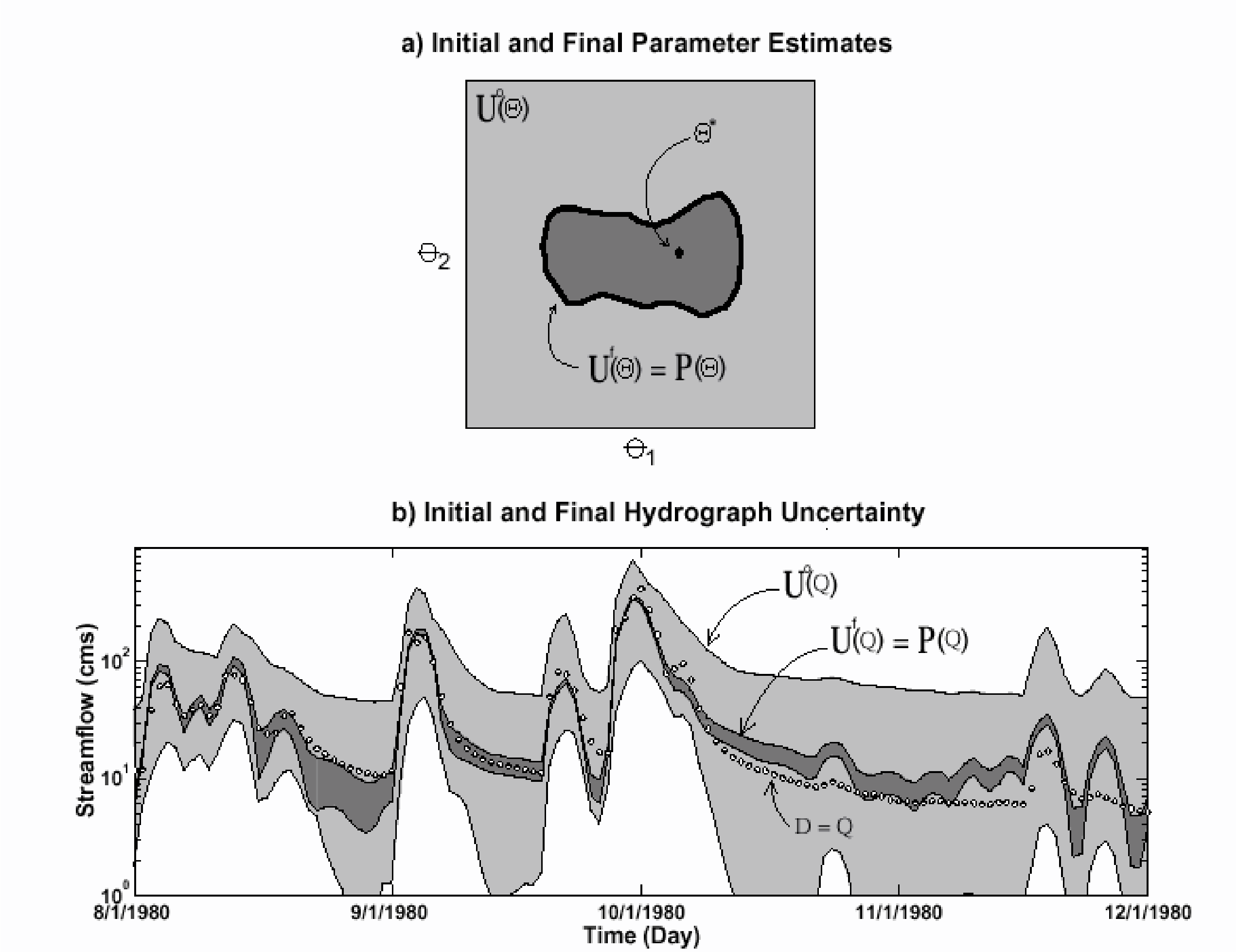
Parameter uncertainty

Multi-objective calibration: Pareto Optimality



Parameter uncertainty

Multi-objective calibration



Parameter uncertainty

<u>Multi-objective calibration: </u>Example

- HBV model
- 3 objective functions

$$N_{LF} = \frac{1}{n}\left(\sum_{i=1}^{n}\left(\ln Q_{s,i} - \ln Q_{o,i}\right)^2\right)$$

$$N_{HF} = \frac{1}{n}\left(\sum_{i=1}^{n}\left(Q_{s,i} - Q_{o,i}\right)^2\right)$$

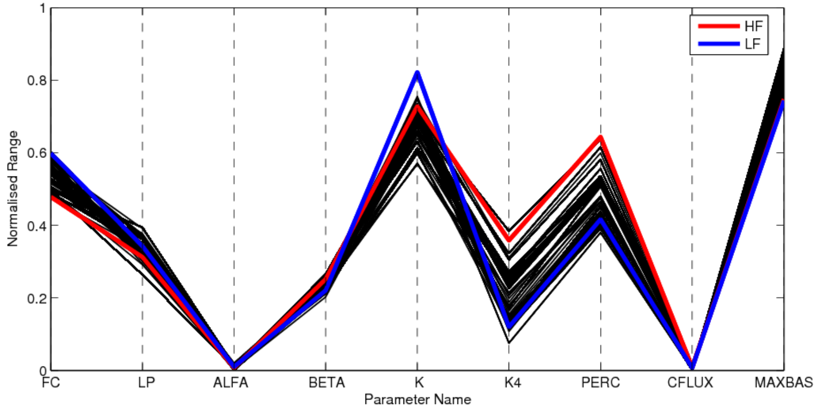
$$N_{GW} = 1 - R = 1 - \frac{\sum_{i=1}^{n}\left(W_{s,i} - \overline{W}_s\right)\cdot\left(W_{o,i} - \overline{W}_o\right)}{\sqrt{\sum_{i=1}^{n}\left(W_{s,i} - \overline{W}_s\right)^2 \cdot \sum_{i=1}^{n}\left(W_{o,i} - \overline{W}_o\right)^2}}$$

Parameter uncertainty

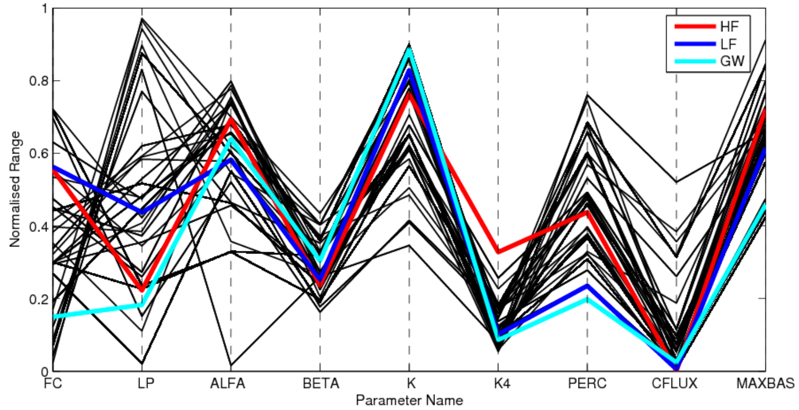
Multi-objective calibration: Example

Parameter ranges

N_{HF} and N_{LF}



N_{HF}, N_{LF} and N_{WT}

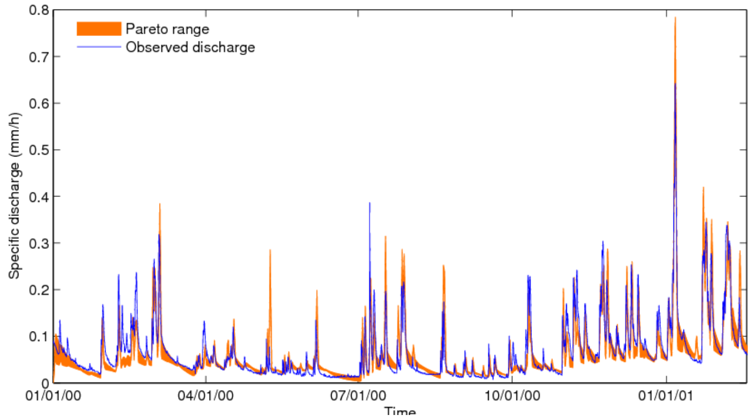


Parameter uncertainty

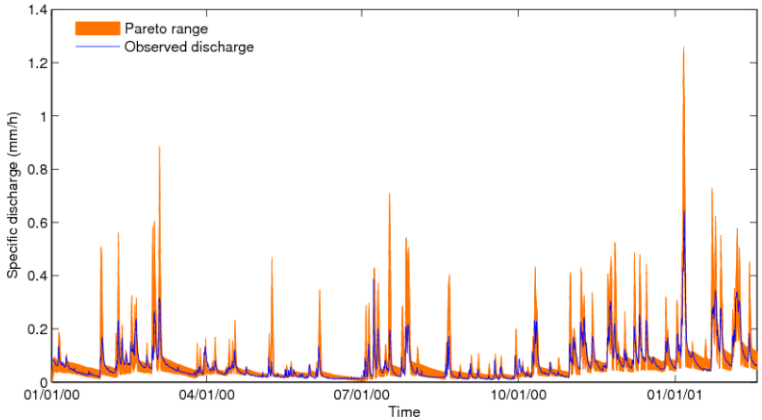
Multi-objective calibration: Example

Hydrograph

N_{HF} and N_{LF}



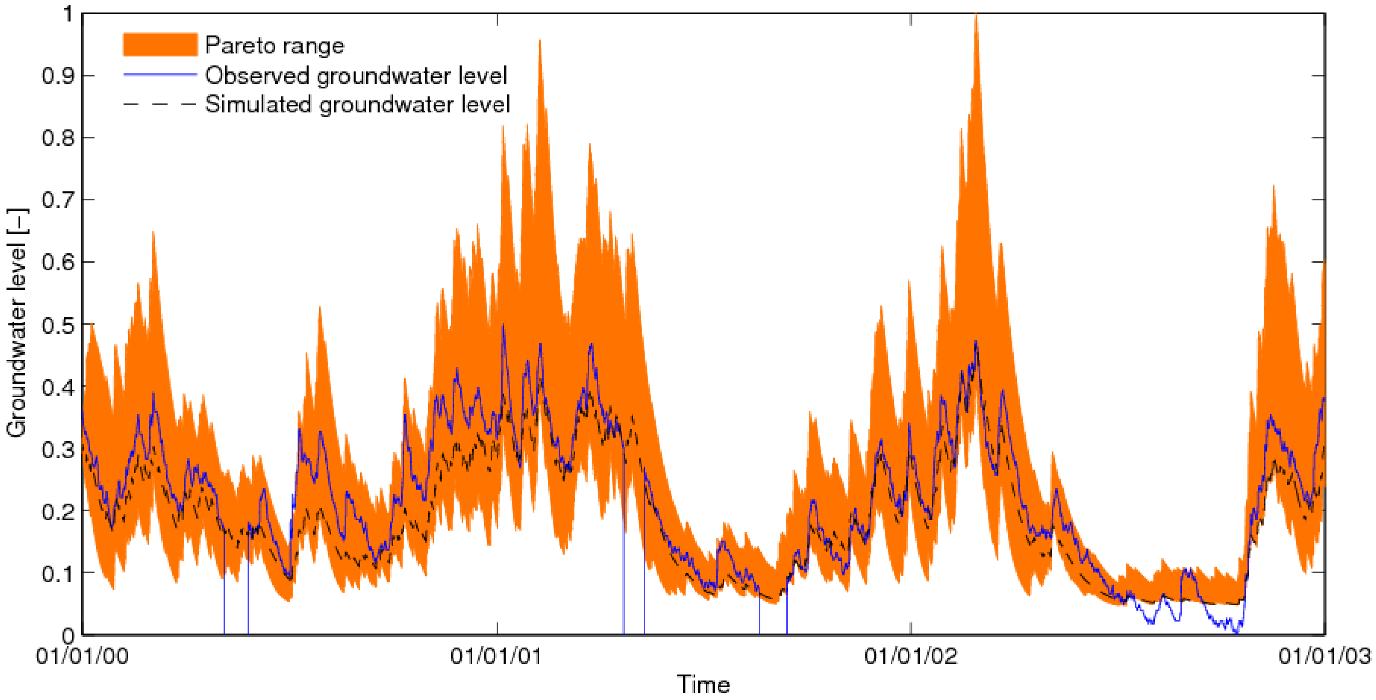
$N_{HF,}$ N_{LF} and N_{WT}



Parameter uncertainty

Multi-objective calibration: Example

Groundwater table



Parameter uncertainty

Multi-objective calibration

- Takes into account the multi-objective nature of the calibration problem
- Takes into account that different parts of the hydrograph can be subject to different error processes
- Reflects the model's inability to correctly and simultaneously simulate different aspects of the simulations

Stepped Calibration Approach

(1) Select different specific characteristics of the time series that should be well simulated, e.g. high and low flow.

(2) Associate model parameters with the selected characteristics

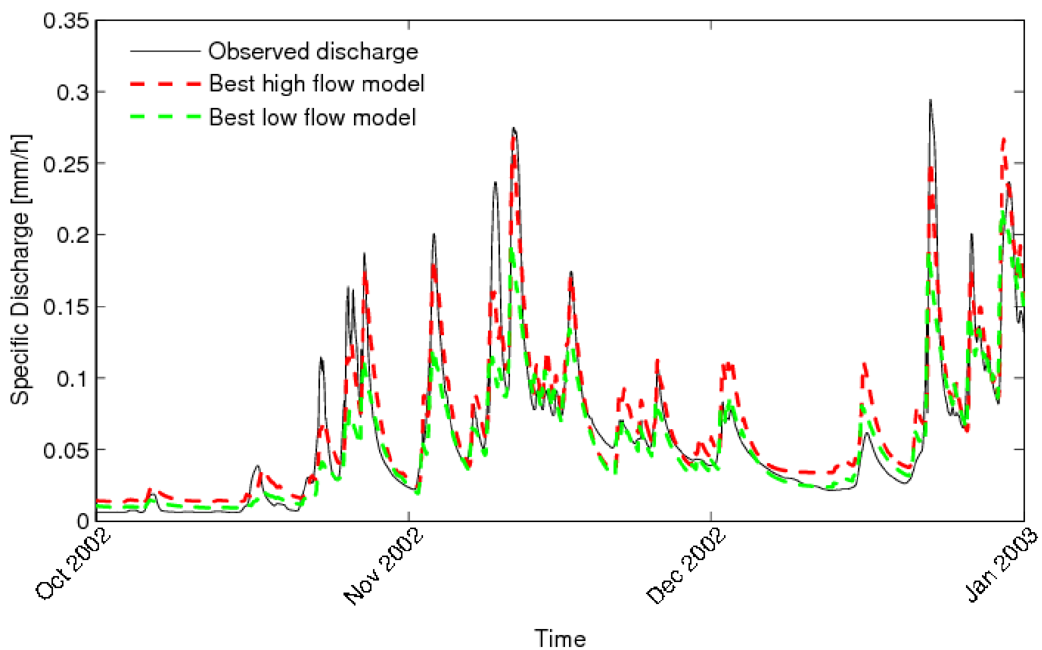
(3) Define objective functions that represent performance measures for modelling the selected characteristics

(4) Calibrate each group of parameters associated with each objective function individually, while fixing the remaining parameters at constant values

Stepped Calibration Approach

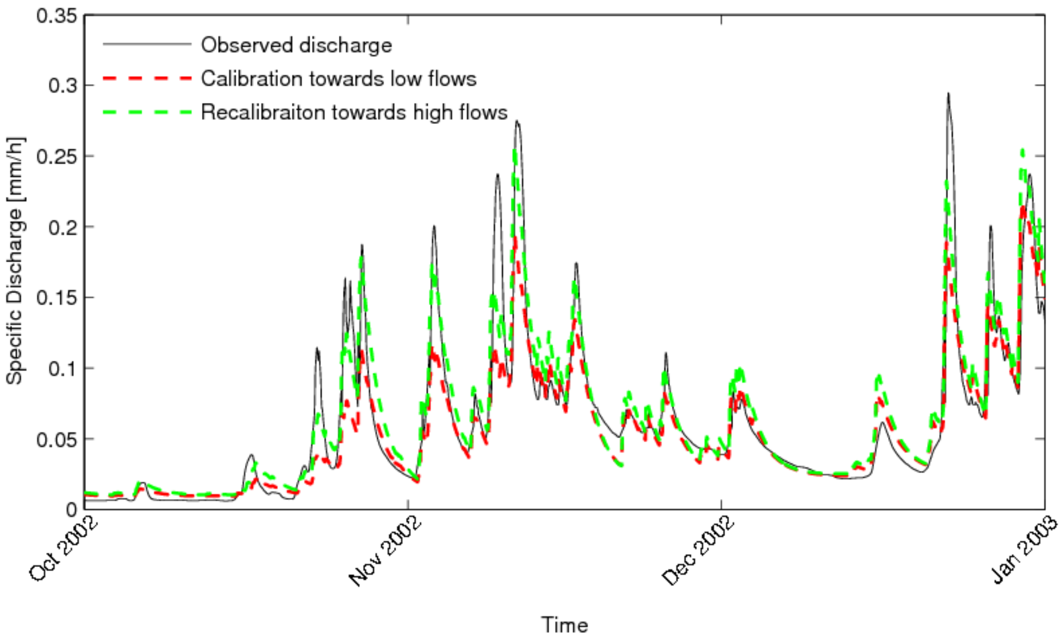
Example:

- Calibration of stream flow with respect to high and low flows, i.e. NS and logNS
- The optimal models related to two objective functions are different and both unrealistic



Stepped Calibration Approach

Example:
First calibrate the groundwater related parameters, i.e. low flow, and then the others. The baseflow simulation remains almost unchanged



Stepped Calibration Approach

- Recognizes that results obtained by single objective calibration can be unrealistic
- Tries to emulate the steps followed by hydrologists in manual calibration
- Provides a balanced, physically realistic solution

Dynamic Identifiability Analysis

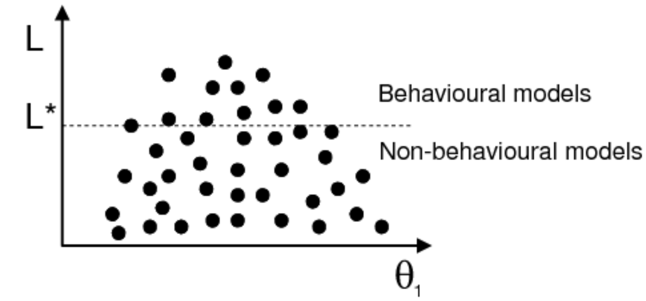
Analyses parameter identifiability in a moving time window:

(1) allows analysing how different regimes influence identifiability of model parameters

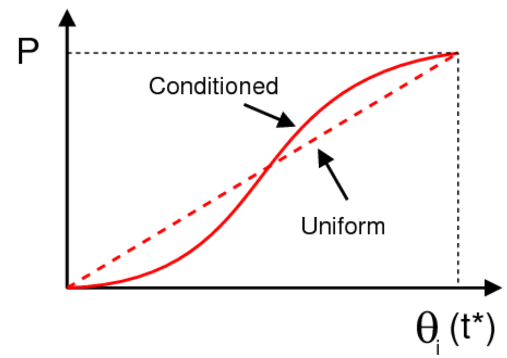
(2) allows investigating the assumption that model parameters are constant in time

Dynamic Identifiability Analysis

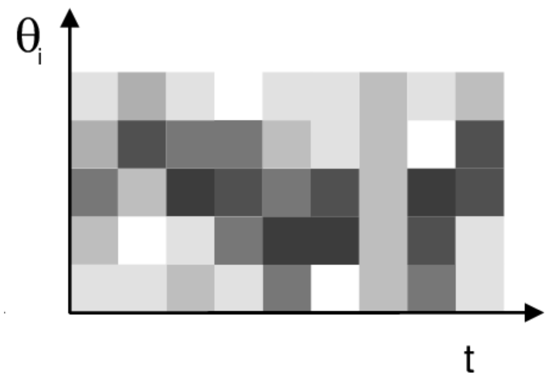
(1) Sample feasible parameter space



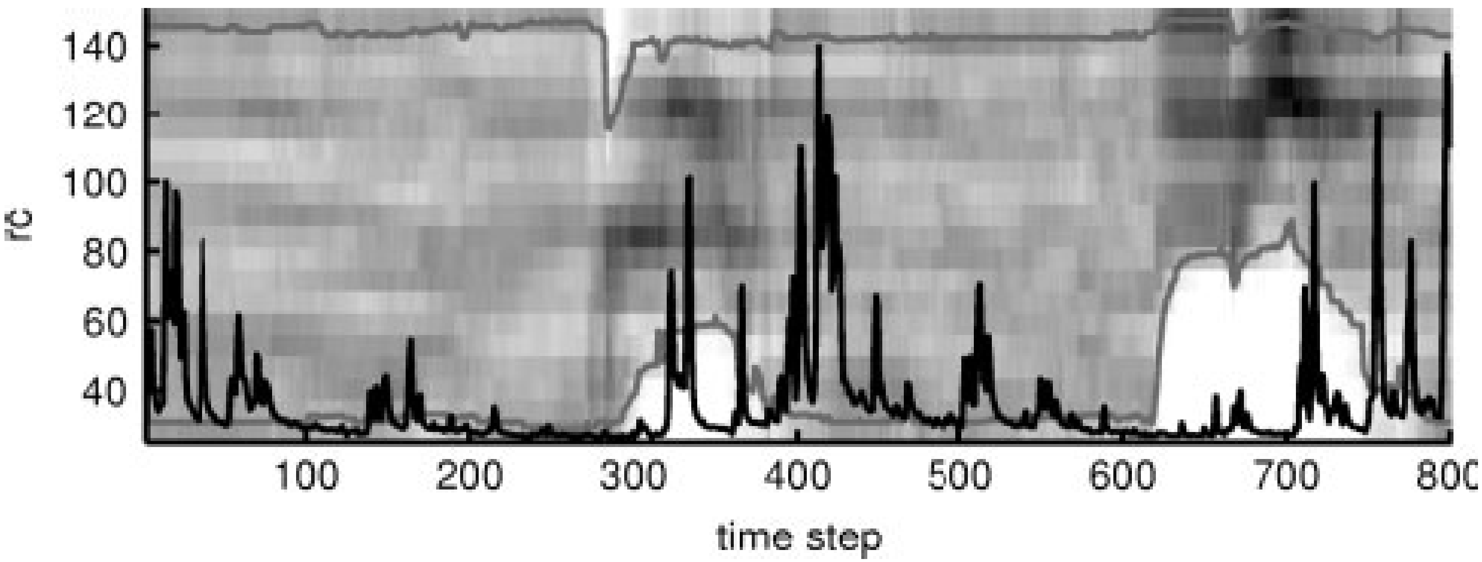
(2) Construct cumulative parameter distribution functions



(3) Evaluate parameter identifiability for each time step



Dynamic Identifiability Analysis

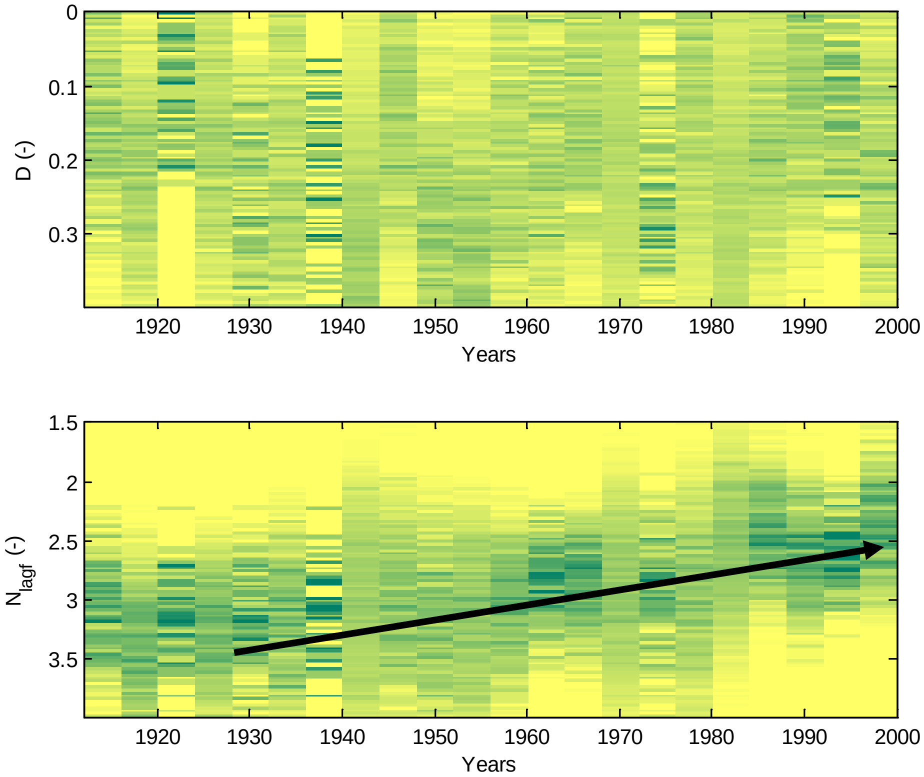


- ✓ Objectives
- ✓ Sources of uncertainty
- ✓ Why do we care?
- ✓ Calibration
- ✓ Objective functions
- ✓ Optimization
- ✓ Parameter uncertainty

New approaches

What have we learned?

Dynamic Identifiability Analysis



Parameter N_{lagf}, which represents the lag time of the system, is non-stationary, i.e. it decreases with time

Dynamic Identifiability Analysis

- It allows analyses of parameter identifiability in time
- It is useful to enhance model structural limitations
- It can help to detect regimes with higher information content than others for specific parameters

Current view on model evaluation

- Requirements for model application:
  - Model parameters have to be well identifiable
  - The model has to be able to adequately reproduce the observations
  - The model has to be a realistic representation of the natural system
- Requirements for model evaluation:
  - Evaluate the model with respect to the above mentioned aspects
  - Identify the effect of various sources of error on model predictions and parameters

Current state

- At present no unique framework for the evaluation of all aspects related to model evaluation

- Different approaches could be combined based on the requirements of the specific problem