WaZuBay Workshop on Uncertainty Quantification and Calibration

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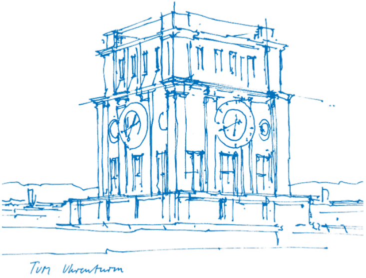
LRZ & TUM (Scientific Computing in Computer Science)



Outline

Uncertainty Quantification (UQ) and Sensitivity Analysis (SA) of Environmental Models

Our framework for UQ & SA

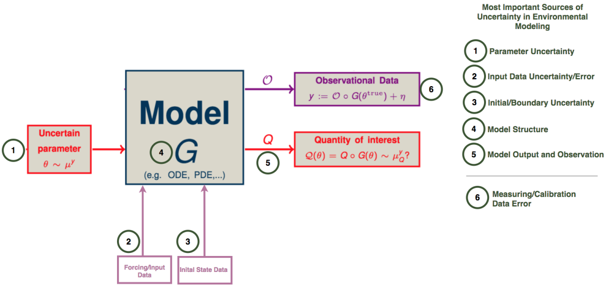
- Algorithms/Mathematical background
- Presentation of some results

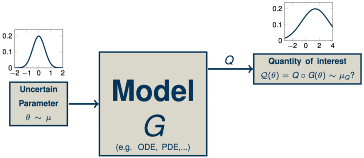
Calibration/Optimization/Inference/Inversion

- Numerical Optimization
- Bayesian approach

Other Software for UQ and Calibration

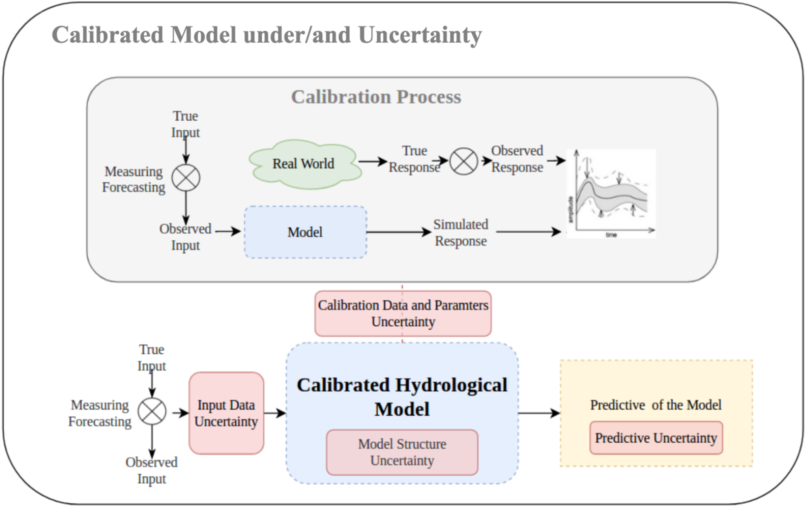
Environmental models & UQ & SA





Environmental models & UQ & SA

Sources of the uncertainty - yet another presentation



Environmental models & UQ & SA II

Reasons for UQ & SA:
Support and complement model calibration!

- Ranking - rank input factors according to the contribution on the output
- Screening - identifying (ir)relevant input factors
- Mapping - relating regions of the inputs and outputs

UQ - Quantifying uncertainty in the output of the model
SA - Apportioning output uncertainty to the different input factors

Our Framework for UQ & SA

Methods for UQ & SA

Sampling Approach
General Polynomial Chaos Expansion Methods (gPCE)
Global Sensitivity Analysis

Sampling Methods - Monte Carlo Sampling

- given a probability distribution $\rho(\boldsymbol{\theta})$
- generate samples using a pseudo-random number generator $\{\boldsymbol{\theta}_i\}_{i=1}^N$
- perform deterministic computations using these samples $f(t, \boldsymbol{\theta}_i) = f_i, i = 1, \ldots, N$
- aggregate the results, e.g., $\mathbb{E}[f(t, \boldsymbol{\theta})] \approx \bar{f} = \frac{1}{N} \sum_{i=1}^N f_i$

- How good is this approximation (on average)?

$$\text{RMSE} := \sqrt{\mathbb{E}\left[(\mathbb{E}[f(t, \boldsymbol{\theta})] - \bar{f})^2\right]} = \frac{\sigma_f}{\sqrt{N}} \approx \frac{\bar{\sigma}_f}{\sqrt{N}} \text{ with } \bar{\sigma}_f^2 = \frac{1}{N-1} \sum_{i=1}^N (f_i - \bar{f})^2$$

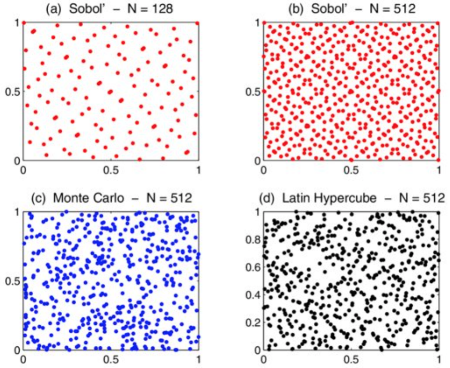
pros

- easy to understand and implement; robust; “embarrassingly” parallel
- convergence rate independent of the input dimension

cons

- convergence rate $\mathcal{O}(\frac{1}{\sqrt{N}}) \rightarrow$ very slow
- no way to “prioritize” some parameter directions

Sampling Methods - Different (Statistical) Sampling Strategies



- General idea: produce samples that are “well” spaced
- Latin hypercube sampling, Sobol sequence, Halton sequence... [Caflisch et al. 1998]
- Caution: Transformation from the original samples to parameter values needed

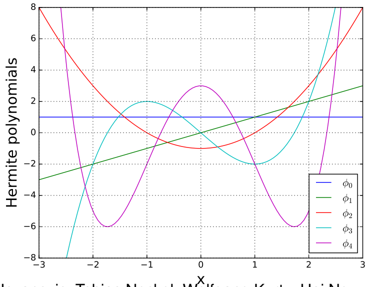
General Polynomial Chaos Expansion I

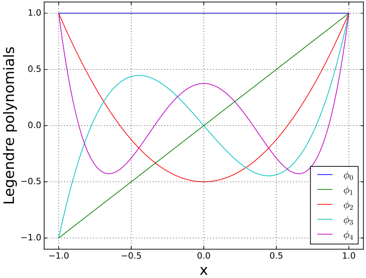
- Approximate a random variable $f(t,\theta)$ by truncated series expansion of orthogonal polynomials (analogy with Fourier series) [Xiu and Karniadakis 2002]

$$f(t,\theta) = \sum_{n=0}^{\infty} \hat{f}_n(t)\,\phi_n(\theta) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\,\phi_n(\theta) \tag{1}$$

- **type of polynomials chosen w.r.t. parameter distribution** $\rho(\theta)$
- exploit orthonormality of the underlying basis

$$\hat{f}_n(t) = < f(t,\theta), \phi_n(\theta) >_\rho = \int_\Omega f(t,\theta)\,\phi_n(\theta)\,\rho(\theta)\,d\theta \tag{2}$$





General Polynomial Chaos Expansion II

$$f(t,\theta) \approx \sum_{n=0}^{N-1} \hat{f}_n(t)\, \phi_n(\theta) \tag{3}$$

Compute statistical properties of QoI

$$E[f(t,\theta)] \approx \hat{f}_0(t) \tag{4}$$

$$Var[f(t,\theta)] \approx \sum_{n=1}^{N-1} \hat{f}_n^2(t) \tag{5}$$

The Pseudo-spectral Method

- Use quadrature rule to compute coefficients [Conrad and Marzouk 2012; Constantine, Eldred, and Phipps 2012]

$$\hat{f}_n(t) = \sum_{k=0}^{K-1} f(t,x_k)\, \phi_n(x_k)\, w_k \tag{6}$$

- nodes, weights $\{x_k, w_k\}_{k=0}^{K-1}$ chosen w.r.t. the input probability distribution $\rho(\theta)$
- evaluate the forward model $f(t,\theta)$ at each x_k!

General Polynomial Chaos Expansion III
The Pseudo-spectral Method

- Ideally, the projection and the quadrature rule are as **accurate and efficient** as possible $\Rightarrow$ using **the least number** of nodal points/deterministic forward simulations
- From 1-d to *d*-dimensional space via tensor product formulations $\Rightarrow$ exponential growth with parameter dimensionality

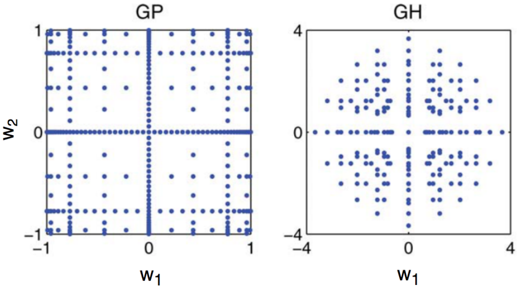


Figure: (left) level five (321 nodes) Gauss-Patterson (GP) sparse grid for uniformly distributed variables; (right) level five (181 nodes) Gauss- Hermite (GH) sparse grid for standardized normally distributed variables

Sensitivity Analysis

Problem

- How sensitive is $f(t, \boldsymbol{\theta})$ (or some other QoI) to changes in $\boldsymbol{\theta} \in \boldsymbol{X}$?
- What is the relative contribution of $\theta_i, i = 1, \ldots, d$ to the output uncertainty?

Local sensitivity analysis

- asses the "sensitivity" around some nominal value, e.g. using gradients of output w.r.t. inputs

Global sensitivity analysis

- based on analyzing a suitable "measure" of uncertainty, e.g. the variance

One-at-Time (OAT) vs. All-at-Time (AAT)

Time-varying vs. Aggregation over-time

Global Variance-based Sensitivity Analysis

Sobol' Indices (SI) [Bauwens, Nossent, and Elsen 2011; Saltelli et al. 2010]

- Underlying assumption: input composed of **independent** random variables $\boldsymbol{\rho}(\boldsymbol{\theta}) = \prod_{i=1}^{d} \rho_i(\theta_i)$
- Total variance decomposition $\mathrm{Var}[f(t,\boldsymbol{\theta})] = \sum_{i=1}^{d} V_i(t) + \sum_{1\leq i<j\leq d} V_{ij}(t) + \ldots + V_{12..d}(t)$

First order SI

fraction of the model output variance that would disappear on average if θ_i is fixed

$$S_i(t) \;=\; \frac{Var[E[f|\theta_i]]}{\mathrm{Var}[f(t,\boldsymbol{\theta})]} \;=\; \frac{\mathrm{Var}[f] - E[Var[f|\theta_i]]}{\mathrm{Var}[f]} \;=\; \frac{V_i(t)}{\mathrm{Var}[f]} \tag{7}$$

Total order SI evaluate the total effect of an input parameter

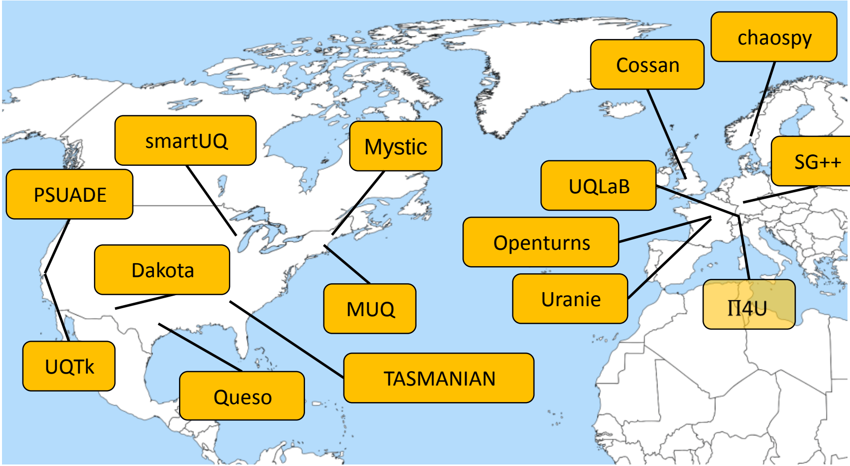
$$S_i^T(t) \;=\; \frac{E[Var[f|\boldsymbol{\theta}_{-i}]]}{\mathrm{Var}[f]} \;=\; \frac{\sum_{n\in A_i} V_n}{\mathrm{Var}[f]} \;=\; 1 \;-\; \frac{V_{-i}(t)}{\mathrm{Var}[f]} \tag{8}$$

- Computing by MC samplse $\Rightarrow \#model\_runs = N(d+2)$

SI and gPCE [Sudret 2008]

$$S_i^T(t) \;\approx\; \frac{\sum_{n\in A_i} \hat{f}_n^2(t)}{\sum_{n=1}^{N-1} \hat{f}_n^2(t)} \tag{9}$$

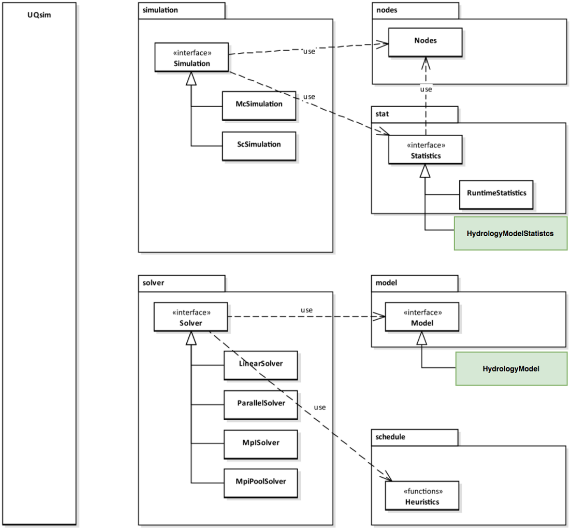
World of UQ Software - No need to code from scratch



source of world map: http://en.wikipedia.org

SIAM conference UQ 18, minisymposia 88, 102, 115, and 128: Software for UQ, Tobias Neckel & Dirk Pflüger
see also `https://www5.in.tum.de/wiki/index.php/SIAMUQ18_-_Slides_Minisymp_Software4UQ`

Sketch of our In-house software solution



Our software relies on Chaospy library, UQEF library KÃ¼nzner 2021, and other Python libraries (e.g., mpi4py, Pandas, Plotly)

Our Framework for UQ & SA - Functionalities

Comprehensive (time-varying) uncertainty quantification and sensitivity analysis of hydrological models

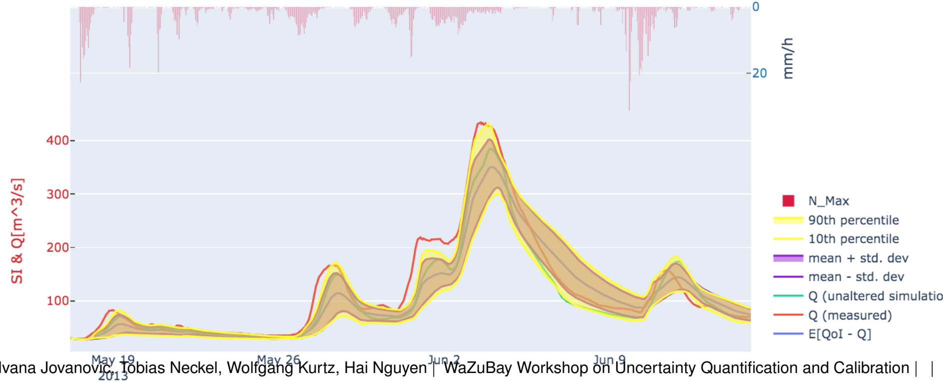
Functionalities:

- MC and Quasi-MC sampling (e.g., Halton, Sobol, Latin Hypercube...)
- Generalized Polynomial Chaos (gPCE)
  - Transformation - from dependent variables to independent,
    Introduction of the auxiliary variables, Rosenblatt transformation, Cholesky, etc.
  - Point collocation method
  - Pseudo-spectral projection
- Sensitivity Analysis
  - Local, gradient-based analysis
  - Global Variance-based - Sobol Indices
  - Global active scores indices
- Definition of Quantity of interest (QoI)
  - Temporally varying QoI (e.g., discharge)
  - Some goodness-of-fit (i.e., NSE, RMSE) summing up the whole period, or computed in the sliding window manner

Visualization of the results I

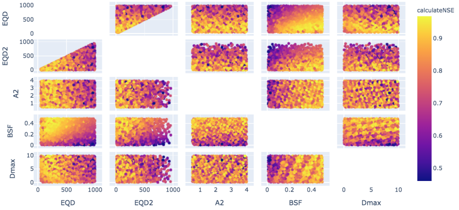
Time-varying influence of 5 parameters on model predictions under the high-flow conditions

- **QoI:** Hourly discharge values
- **Method:** gPCE (Gauss-Legendre quadrature) $q = 7; p = 6$
- **#model evaluations:** 32768
- **Computation time:** $\sim$ 4 hours on 4 compute nodes (28CPU+55GB RAM per node)

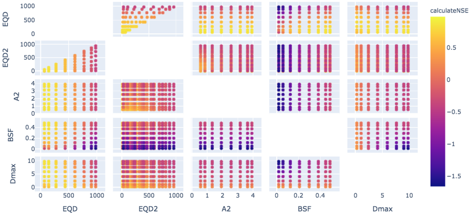


Visualization of the results II

Time-varying influence of 5 parameters on model predictions under the high-flow conditions - Parameters vs. GoF

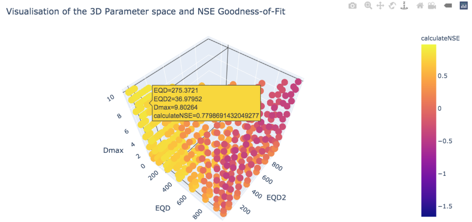


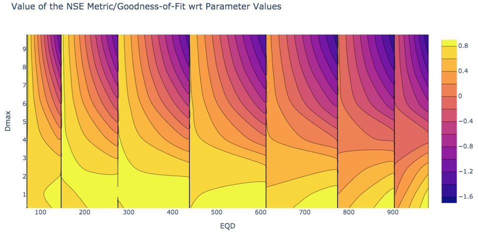
Univariate and bivariate marginal distributions of the parameters - NSE



Visualization of the results III

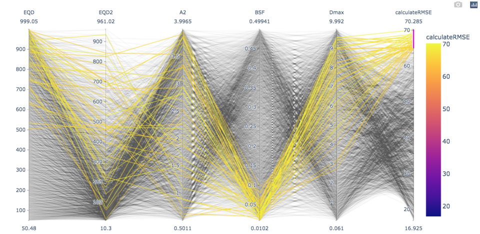
Time-varying influence of 5 parameters on model predictions under the high-flow conditions - Parameters vs. GoF

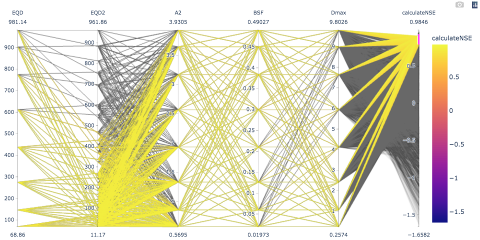




Visualization of the results IV

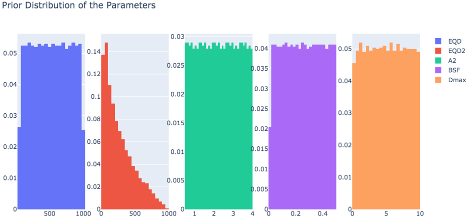
Time-varying influence of 5 parameters on model predictions under the high-flow conditions - Parameters vs. GoF

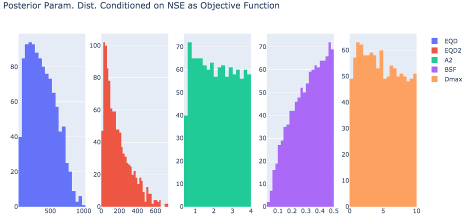




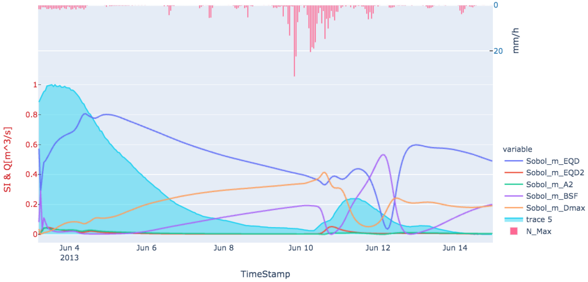
Visualization of the results V

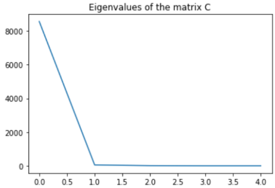
Time-varying influence of 5 parameters on model predictions under the high-flow conditions - Parameters prior and "posterior" distribution

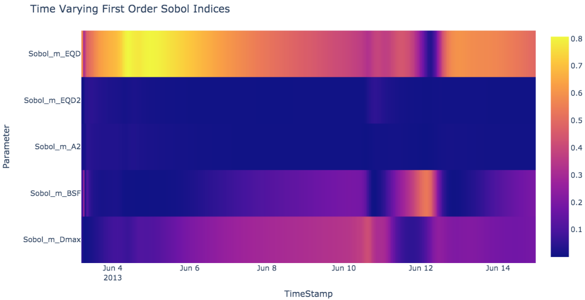




Visualization of the results VI



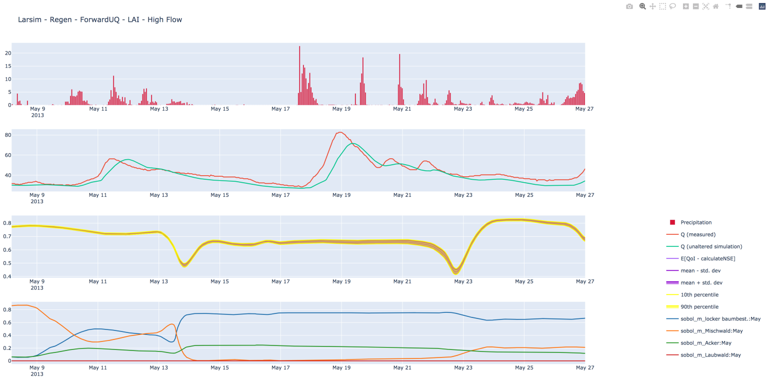




Visualization of the results VII

Time-varying influence of 4 leaf area index parameters on model predictions (QoI-NSE) under the high-flow conditions

- **QoI:** 10-days sliding-window NSE
- **Method:** gPCE (Gauss-Legendre quadrature) $q = 7; p = 6$
- **#model evaluations:** 4096
- **Computation time:** $\sim$ 1.5 hour on 4 compute nodes (28CPU+55GB RAM per node)



Other Methods for UQ & SA in Hydrology

- Variogram Analysis of Response Surfaces (VARS Tool) [Gupta and Razavi 2018; Razavi 2016]
- Distribution-based sensitivity analysis - PAWN & Sensitivity Analysis For Everybody - A Matlab toolbox for Global Sensitivity Analysi - SAFE [Pianosi, Sarrazin, and Wagener 2015; Pianosi and Wagener 2018]
- Fourier based sensitivity analysis - FAST

Conclusions we draw from Forward UQ and SA

- Useful prior calibration tool - help inform important modeling decisions (e.g., parameterization and objective function formulation)
- We built surrogate models in the parameter space, e.g., gPCE or Active Subspaces

How to use what we have learned so far for the further steps - calibration

Calibration - Optimization ...
... Inference - Inversion - Parameter Estimation

Numerical Optimization - Parameter Estimation - Regularized inversion

PEST [John E Doherty and Hunt 2010, doherty2015pest]
PEST++ [Welter et al. 2012]
pyEMU [White, Fienen, and John E. Doherty 2016]

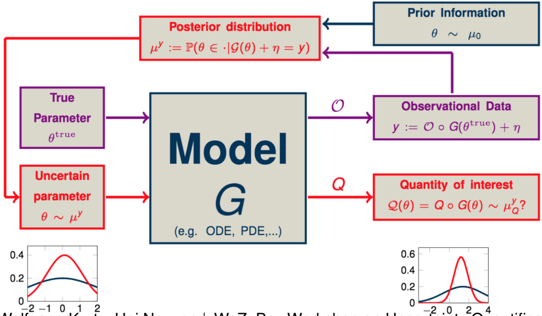
- **Idea:** minimize (multiple) summery (scalar) variables (e.g., measure of model performance, goodness-of-fit, objective function, data misfit, etc.)
- iterative application of the Marquardt-Levenberg minization algorithm
- in each iteration - linearization of the model-parameters to model-output map through Taylor expansion $G \approx \mathbb{X}\boldsymbol{\theta}$ (Jacobian hidden in $\mathbb{X}$)
- convergence criteria - value of some objective function

$$\underbrace{\Phi(\boldsymbol{\theta};\boldsymbol{y})}_{data-misfit} = \frac{1}{2}\|\boldsymbol{\eta}\|_{\Sigma_{\boldsymbol{\eta}}^{-1}} = \frac{1}{2}\|\Sigma_{\boldsymbol{\eta}}{}^{-\frac{1}{2}}(\boldsymbol{y} - \mathbb{X}\boldsymbol{\theta})\|_2^2$$

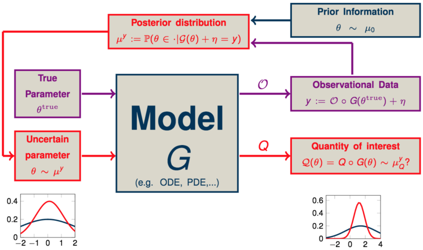
A Statistical Parameter Optimization Tool for Python (SPOTPY) [Houska et al. 2015]

Bayesian Inference (Calibration Under Uncertainty) I

- **Question:** How to initially model the uncertainty in parameters?
- **Idea behind Bayesian Inversion:** For past/collected data $\Rightarrow$ model the uncertainty in model parameters - **exactly the definition of calibration under uncertainty!**
- Potential confusion: Forward UQ vs. Inversion under Uncertainty; what comes first (chicken-or-egg question)?



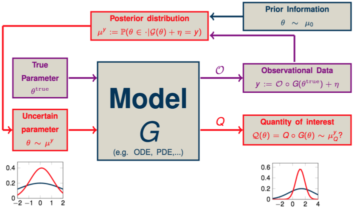
Bayesian Inference (Calibration Under Uncertainty) II



Key-Component - Bayes' Theorem: Combine the prior distribution and the likelihood (observed data and the forward model) to derive the posterior density

$$\pi^y(\theta) = \frac{L(\theta|\mathbf{y}))\pi_0(\theta)}{\int_X L(\theta|\mathbf{y})\pi_0(\theta)d\theta} = \frac{L(\theta|\mathbf{y}))\pi_0(\theta)}{Z(y)} \qquad \pi^y(\theta) \propto L(\theta|\mathbf{y})\pi_0(\theta) \tag{10}$$

Bayesian Inference (Calibration Under Uncertainty) III



Key-Component - Bayes' Theorem:

$$\pi^{\boldsymbol{y}}(\theta) = \frac{L(\theta|\boldsymbol{y}))\pi_0(\theta)}{\int_X L(\theta|\boldsymbol{y})\pi_0(\theta)d\theta} = \frac{L(\theta|\boldsymbol{y}))\pi_0(\theta)}{Z(\boldsymbol{y})} \qquad \pi^{\boldsymbol{y}}(\theta) \propto L(\theta|\boldsymbol{y})\pi_0(\theta)$$

Sequential nature of the Bayesian Inference $\pi_j^{\boldsymbol{y}}(\theta) = \frac{\pi_{j-1}^{\boldsymbol{y}}(\theta)\frac{L_j(\theta|\boldsymbol{y})}{L_{j-1}(\theta|\boldsymbol{y})}}{\frac{Z_j(\boldsymbol{y})}{Z_{j-1}(\boldsymbol{y})}}$

Forward UQ after Bayesian Calibration:

$$\mathbb{E}_{\pi^{\boldsymbol{y}}}[\mathcal{Q}] = \frac{1}{Z(y)} \int_X \mathcal{Q}(\theta)L(\theta|\boldsymbol{y})\pi_0(\theta)d\theta = \frac{\mathbb{E}_{\pi_0}[\mathcal{Q}(\cdot)L(\cdot|\boldsymbol{y})]}{\mathbb{E}_{\pi_0}[L(\cdot|\boldsymbol{y})]} \tag{11}$$

Bayesian Inference & MCMC Sampling

- Approximate the posterior through the samples... or use these samples in Forward UQ
- **basic idea**: Construct an ergodic Markov Chain $(\boldsymbol{\theta_n})_{n\geq 1}$ which is stationary w.r.t. π^y
- **input**: likelihood L, prior π_0, proposal distribution q, number of samples M
- **output**: samples $\boldsymbol{\theta_1}, \ldots, \boldsymbol{\theta_M}$

Algorithm 1: Metropolis-Hastings

---

procedureMetropolis Hastings(L, π_0, q, M)
    Choose a starting point θ_0
    for i=1,...,M **do**
        Draw candidate θ' from proposal $q(\cdot|\theta_{i-1})$
        Compute acceptance probability
        $\alpha(\theta', \theta_{i-1}) = min\{1, \frac{q(\theta_{i-1}|\theta')L_y(\theta')\pi_0(\theta')}{q(\theta'|\theta_{i-1})L_y(\theta_{i-1})\pi_0(\theta_{i-1})}\}$
        Set the sample θ_i to
        $\theta_i = \theta'$ with probability $\alpha(\theta', \theta_{i-1})$ (accept); otherwise:
        $\theta_i = \theta_{i-1}$ with probability $1 - \alpha(\theta', \theta_{i-1})$(reject)
    end
    return $\theta_1, \ldots, \theta_M$

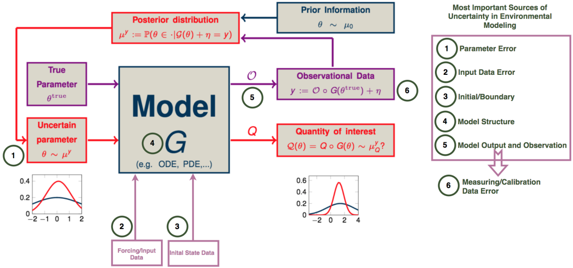
---

https://chi-feng.github.io/mcmc-demo/

Environmental models & Bayesian Inference

- Generalized likelihood uncertainty estimation (GLUE) [Beven and Freer 2001] [Jasper A Vrugt et al. 2009]
- Shuffled Complex Evolution Metropolis algorithm (SCEM-UA)
  - Merging the strengths of: Metropolis algorithm, controlled random search, competitive evolution, and complex shuffling
- DiffeRential Evolution Adaptive Metropolis - DREAM [Jasper A. Vrugt 2016; Jasper A. Vrugt et al. 2013]
  - Subspace sampling and outlier chain correction $\Rightarrow$ speed up convergence to the target distribution

Bayesian Inversion for Complex Models



I Choosing the adequate error model

The assumption about independent and identically distribute error with standard Gaussian distribution is not suitable in more complex scenarios

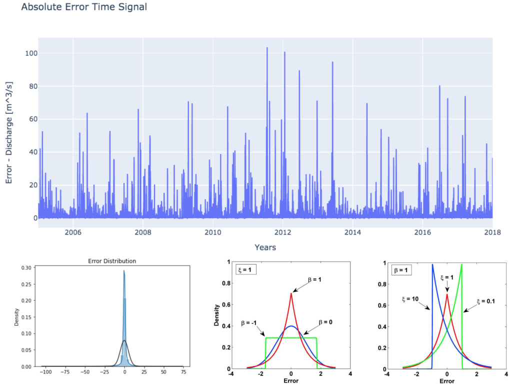
II Accelerating Posterior Exploration

e.g., use of the surrogate models, parallelization of the model runs...

Bayesian Inference for Complex Models

I Choosing the adequate error model

Heteroscedastic (variance dependent on magnitude of data), auto-correlated error model with a more complex (i.e., non-Gaussian) distribution (e.g., Laplacian distribution).



Bayesian Inference for Complex Models

II Accelerating Posterior Exploration

1. Multiple parallel chains [Jasper A. Vrugt 2016]
2. Multi-fidelity methods (e.g., two-stage MCMC) [Eric Laloy, 2013]
3. Methods based on Transport Maps, i.e., pre-conditioning

To conclude...

You heard about:

- Forward UQ and SA
  - Details on our in-house software tool (application: Larsim)
- Calibration - Inversion
  - Numerical Optimization
  - Bayesian Framework

Topic for discussion...
Which methods you use to calibrate the model and get insights into the model parameters? :-)

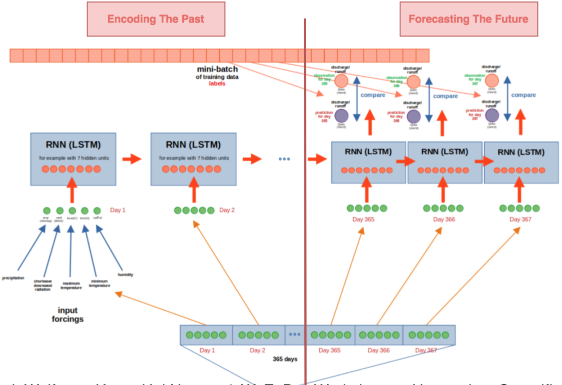
Extra

Bayesian Neural Network for Time-series Forecasting under Uncertainty

Building the Surrogate Model in Data Space

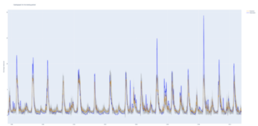
Time-series Forecasting under Uncertainty

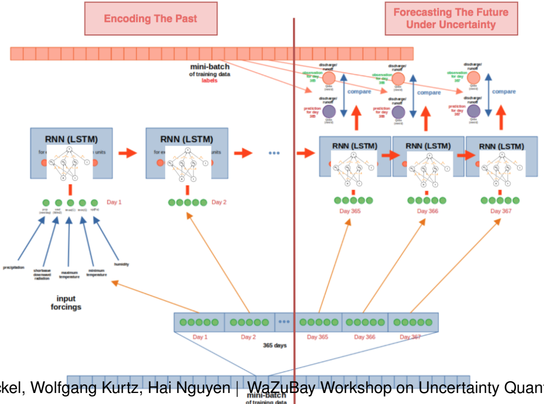
- Data-driven Model - Neural Network as a Surrogate model in Data Space
- Recurrent neural network (RNN) -> Long short-term memory (LSTM) [Hochreiter and Schmidhuber 1997; Kratzert, Klotz, Brenner, et al. 2018; Kratzert, Klotz, Shalev, et al. 2019]
- Necessary Adaptations for the Prediction of the Discharge Time-series



Time-series Forecasting under Uncertainty

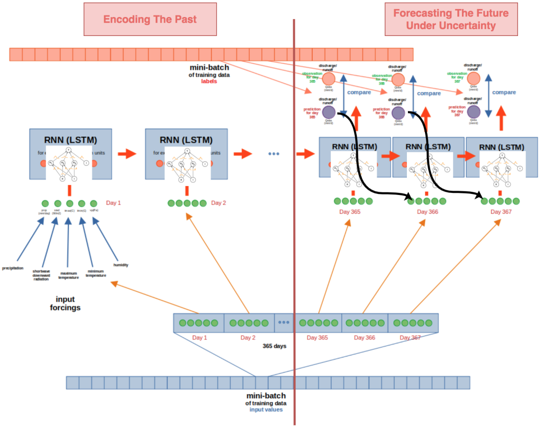
- **When Bayes enters the game** [Blundell et al. 2015]





Time-series Forecasting under Uncertainty

- Spicing up things even further



Time-series Forecasting under Uncertainty - Results

Data

- CAMELS Dataset - forcing data for 671 basins in the United States
- Prediction with uncertainty band - peaks are still heavily missed.

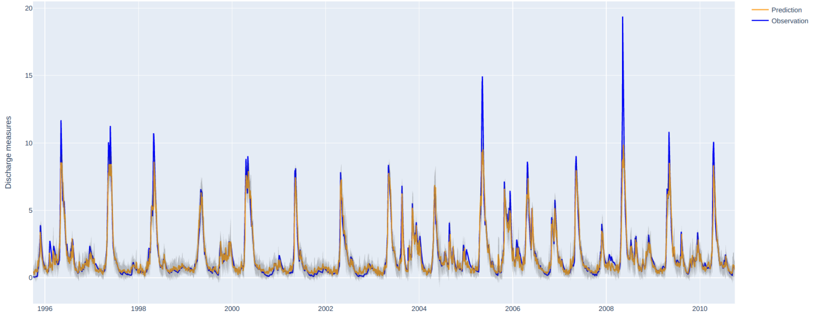


Figure: Hydrograph for the test set predictions (many-to-many) of a catchment in the New England region in the north-east (catchment id: 01013500). The region depicted in gray represents the prediction interval.

Time-series Forecasting under Uncertainty - Results

Data

- LARSIM Regen Dataset

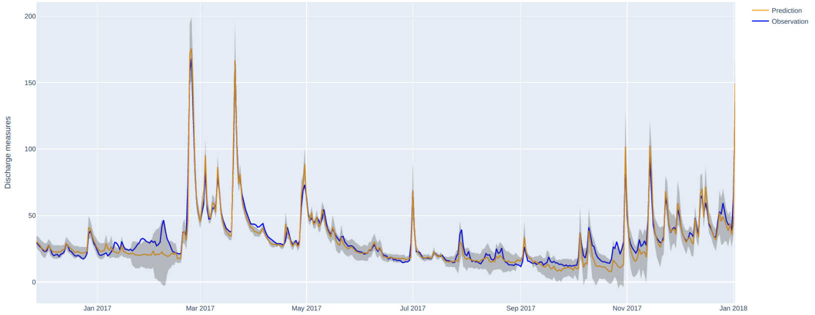


Figure: Hydrograph for Regen catchment - (daily resolution). The region depicted in gray represents the prediction interval

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