Uncertainty quantification (UQ) in geotechnical engineering

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Presentation Overview

1. UQ and uncertainty types
2. UQ framework and components
3. How to consider Uncertainties into UQ framework
4. Final goal of UQ
5. Future considerations

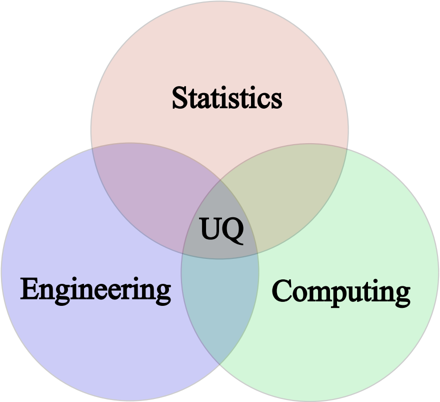
What is Uncertainty Quantification (UQ)?

All models are wrong, but some are useful.
–George E.P. Box

How inaccurate might the models be?
When are they useful in engineering problems?
How much confidence can we have in model's predictions?

UQ provides a framework answering these questions and making model useful.

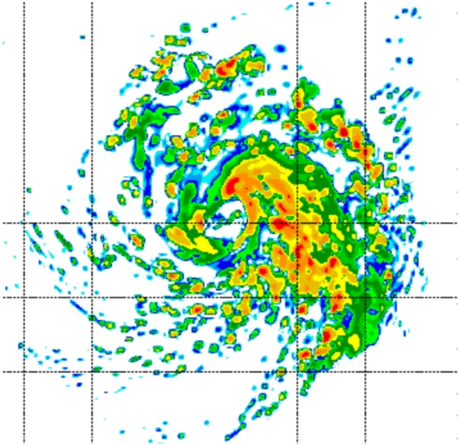
What is Uncertainty Quantification (UQ)?



UQ is the science of quantitative characterization and reduction of uncertainties in both computational and real world applications[1]

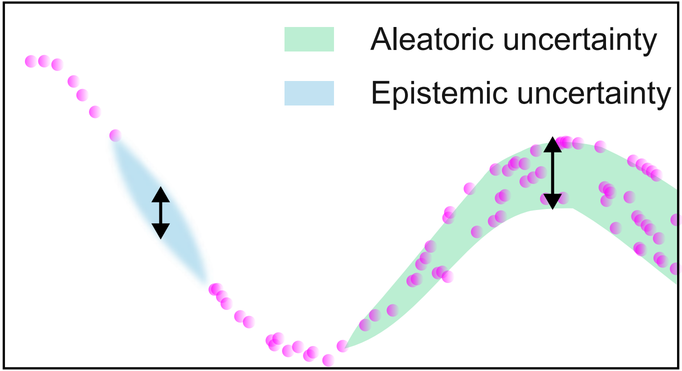
[1] Victor E. Saouma and M. Amin Hariri-Ardebili. “Uncertainty Quantification”. In: *Aging, Shaking, and Cracking of Infrastructures: From Mechanics to Concrete Dams and Nuclear Structures*. Cham: Springer International Publishing, 2021, pp. 423–454.

Unforecast exposures in real world



Wikipedia

sphera.com



Aleatoric uncertainty vs Epistemic uncertainty

Distinguish:

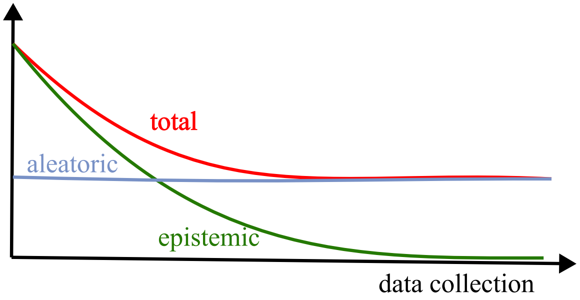
Aleatoric uncertainty

statistical variability, inherently random effects (**irreducible**)

Epistemic uncertainty

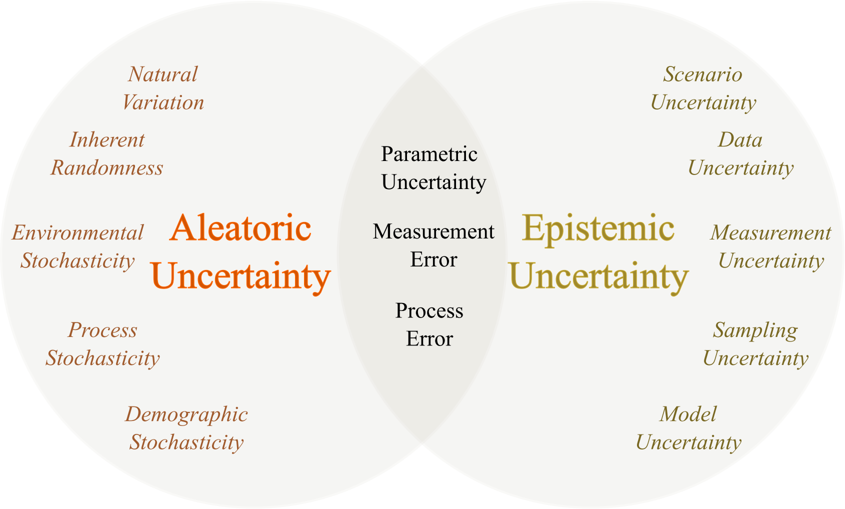
model uncertainty, a lack of knowledge (**reducible**)

Total uncertainty $\approx$ aleatoric uncertainty $+$ epistemic uncertainty

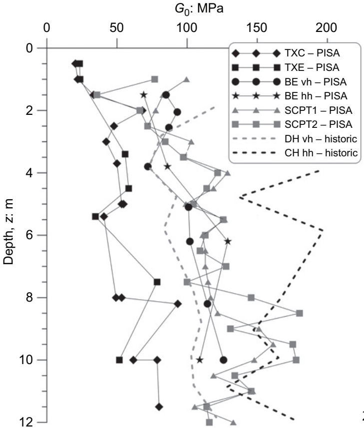


Not simple as it is

Mix of aleatoric and epistemic: Involve too much subjectivity



Examples in geotechnics



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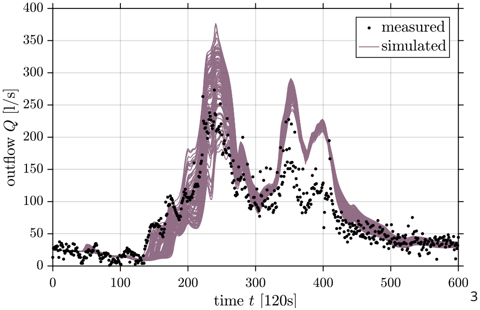

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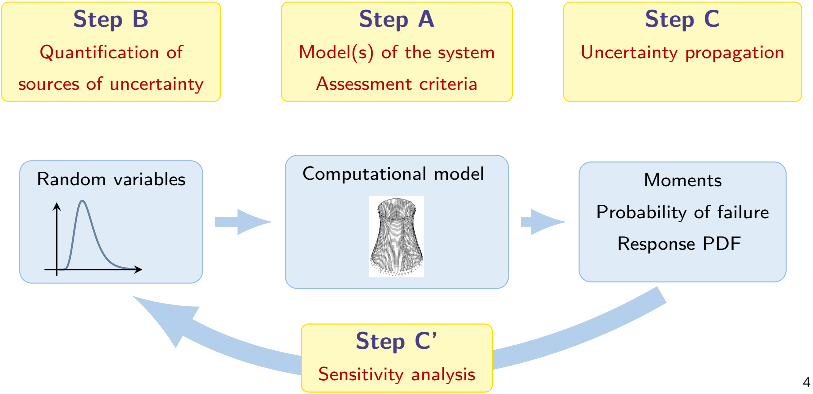
[2] Lidija Zdravković et al. "Ground characterisation for PISA pile testing and analysis". In: *Géotechnique* 70.11 (2020), pp. 945–960.

[3] Joseph B Nagel, Jörg Rieckermann, and Bruno Sudret. "Principal component analysis and sparse polynomial chaos expansions for global sensitivity analysis and model calibration: Application to urban drainage simulation". In: *Reliability Engineering & System Safety* 195 (2020), p. 106737.

UQ framework and components



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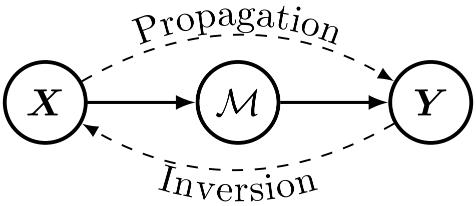
[4] Bruno Sudret. "Uncertainty propagation and sensitivity analysis in mechanical models–Contributions to structural reliability and stochastic spectral methods". In: *Habilitationa diriger des recherches, Université Blaise Pascal, Clermont-Ferrand, France* 147 (2007), p. 53.

UQ framework and components

Two UQ types of problems:



Four components:

1. Model assessment
2. Uncertainty propagation
3. Model calibration
4. Sensitivity analysis

UQ component one-Model assessment

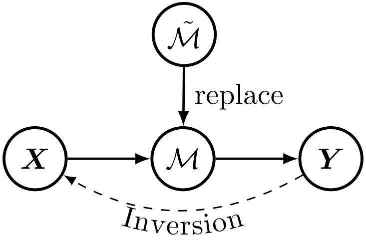
Definition

A computational model $\mathcal{M}$ should contain:

- a mathematical description of the physics
- may be seen as a black box to compute the QoI

- Analytical formula
- Empirical formula
- Packaged programs based on FEM/FDM ...
- $\ldots$

UQ component one-Model assessment



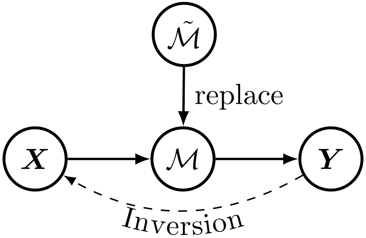
Usage

$$\mathcal{M}(\boldsymbol{x}) \quad \approx \quad \tilde{\mathcal{M}}(\boldsymbol{x})$$

Hours to run seconds to run

- It is built from a limited set of runs of the original model $\mathcal{M}$ called the experimental design $\mathcal{X} = \{\boldsymbol{x}^{(i)}), i = 1, \cdots, N\}$
- It assume some regularity of the model $\mathcal{M}$ and some general functional shape

UQ component one-Model assessment



Some popular choices for $\tilde{\mathcal{M}}$:

Name	Shape	Parameters
Polynomial chaos expansions	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \boldsymbol{y}_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$	$\boldsymbol{y}_{\boldsymbol{\alpha}}$
Low-rank tensor approximations	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \sum_{l=1}^{R} b_l \left(\prod_{i=1}^{M} v_l^i x_i\right)$	$b_l,\ z_{k,l}^i$
Kriging (a.k.a Gaussian processs)	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \boldsymbol{\beta}^T \cdot \boldsymbol{f}(\boldsymbol{x}) + Z(\boldsymbol{x},\omega)$	$\boldsymbol{\beta},\ \sigma_Z^2,\ \boldsymbol{\theta}$
Support vector machines	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \sum_{i=1}^{m} a_i K(\boldsymbol{x}_i,\boldsymbol{x}) + b$	$\boldsymbol{a},\ b$
Neural networks	$\tilde{\mathcal{M}}(\boldsymbol{x}) = f_n\left(\cdots f_2(b_2 + f_1(b_1 + \boldsymbol{w}_1 \cdot \boldsymbol{x}) \cdot \boldsymbol{w}_2)\right)$	$\boldsymbol{w},\ \boldsymbol{b}$

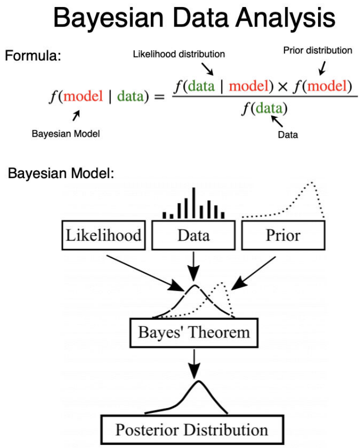
UQ component two-Model calibration

Choice for UQ inversion

Choice for the UQ method is totally based on the **quantity** of accessible data:

- **Lack** or **no** data available, model can be solely based on expert judgement
- **Substantial** volume data available, model can fully use statistical inference (e.g., the methods of moments)
- **Combination** of two above: Bayesian methods

$$\pi(\boldsymbol{x}|\mathcal{Y}) = \frac{\mathcal{L}(\boldsymbol{x}|\mathcal{Y}) \cdot \pi(\boldsymbol{x})}{\pi(\mathcal{Y})}$$



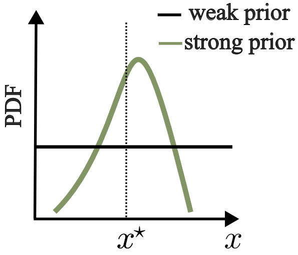
From Matt Dancho

UQ component two-Model calibration

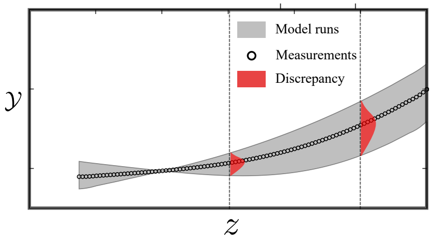
Bayesian methods

Expert guess + Limited data $\rightarrow$ Distribution

Prior:



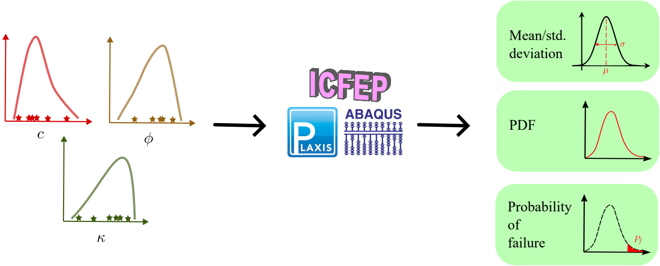
Likelihood:



Notable caveats:

- Prior-Requires specific expertise
- Likelihood-Computationally expensive

UQ component three-Uncertainty propagation



- Output statistics, i.e., mean, standard deviation. etc.

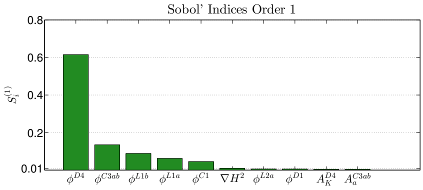
$$\mu_{\boldsymbol{Y}} = \mathbb{E}_{\boldsymbol{X}}[\mathcal{M}(\boldsymbol{X})];\ \sigma^2_{\boldsymbol{Y}} = \mathbb{E}_{\boldsymbol{X}}[(\mathcal{M}(\boldsymbol{X}) - \mu_{\boldsymbol{Y}})^2]$$

- Distribution of the QoI

- Probability of exceeding an admissible threshold y_{adm} following $P_f = \mathbb{P}(\boldsymbol{Y} \geq y_{adm})$

Sensitivity analysis-Determine what are the input parameters whose uncertainty explains the variability of the QoI

- detect input parameters whose uncertainty has no impact on the output variability
- detect input parameters which allow one to best decrease the output variability when set to a deterministic value
- detect interactions between parameters



Variance decomposition (Sobol' indices)

UQ component four-Sensitivity analysis

Total variance:

$$D \equiv \text{Var}[\mathcal{M}(\boldsymbol{X})] = \text{Var}[\sum_{u \subset \{1,\cdots,M\}} \mathcal{M}_u(\boldsymbol{X}_u)] = \sum_{u \subset \{1,\cdots,M\}} \text{Var}[\mathcal{M}_u(\boldsymbol{X}_u)]$$

- Sobol's indice:

$$S_u \stackrel{\text{def}}{=} \frac{\text{Var}[\mathcal{M}_u(\boldsymbol{X}_u)]}{D}$$

- First-order Sobol's indice:

$$S_i = \frac{D_i}{D} = \frac{\text{Var}[\mathcal{M}_i(\boldsymbol{X}_i)]}{D}$$

  Quantify the effect of each input parameter separately
- Total Sobol's indice:

$$S_i^T \stackrel{\text{def}}{=} \sum_{u \supset i} S_u$$

  Quantify the total effect of x_i, including interactions with other variables

Uncertainty quantification for engineering problems

Research topics

- Uncertainty modelling for engineering systems
- Bayesian model calibration
- Structural reliability analysis
- Surrogate models (low dimensions/high dimensions)
- Stochastic inverse problem
- Global sensitivity analysis
- Reliability-based design optimization
- ...

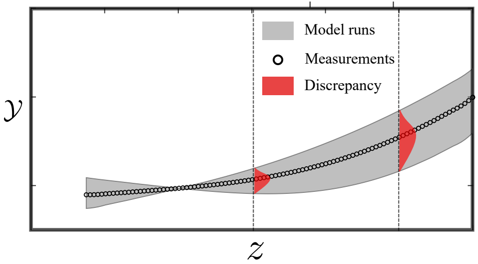
Connecting physics with FE modelling

Through an additive observation error:

$$\boldsymbol{y} = \mathcal{M}(\boldsymbol{x}) + \boldsymbol{\varepsilon} \quad (1)$$

The rationale behind the equation:

- Assume observation error ε is additive
- Assume ε Gaussian form



$$\text{Real physics} \xrightarrow{\delta} \text{Computational Model } \mathcal{M}(x) \xrightarrow{\eta} \text{Surrogate } \tilde{\mathcal{M}}(x)$$

Other uncertainties?

- Observation error $\boldsymbol{\varepsilon}$
- Model discrepancy $\delta(\boldsymbol{x})$
- Numerical/truncation error $\eta(\boldsymbol{x})$

Revised:

$$\begin{aligned} \boldsymbol{y} &= \mathcal{M}(\boldsymbol{x}) + \delta(\boldsymbol{x}) + \boldsymbol{\varepsilon} \\ &= \tilde{\mathcal{M}}(\boldsymbol{x}) + \eta(\boldsymbol{x}) + \delta(\boldsymbol{x}) + \boldsymbol{\varepsilon} \end{aligned}$$

Question: where should the uncertainties go to?

$$\pi(\boldsymbol{x}|\mathcal{Y}) = \frac{\mathcal{L}(\boldsymbol{x}|\mathcal{Y}) \cdot \pi(\boldsymbol{x})}{\pi(\mathcal{Y})} = \frac{\mathcal{L}(\boldsymbol{x}|\mathcal{Y}) \cdot \pi(\boldsymbol{x})}{\int_{\mathcal{D}_{\boldsymbol{X}}} \pi(\boldsymbol{x})\pi(\mathcal{Y}|\boldsymbol{x})\mathrm{d}\boldsymbol{x}}$$

Incorporate uncertainties into $\mathcal{L}(x|\mathcal{Y})$

If only consider observations error ε

$$\boldsymbol{y}_i = \tilde{\mathcal{M}}(\boldsymbol{x}) + \boldsymbol{\varepsilon}, i = 1, \cdots, k;\ \boldsymbol{\varepsilon} \in \mathcal{N}(\boldsymbol{\varepsilon}|\mathbf{0}, \boldsymbol{\Sigma})$$

$$\begin{aligned}
\mathcal{L}(\boldsymbol{x}|\mathcal{Y}) &= \prod_{i=1}^{k} N(\boldsymbol{y}_i|\tilde{\mathcal{M}}(\boldsymbol{x}), \boldsymbol{\Sigma}) \\
&= \prod_{i=1}^{k} \frac{1}{\sqrt{(2\pi)^N \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}\left(\boldsymbol{y}_i - \tilde{\mathcal{M}}(\boldsymbol{x})\right)^{\mathsf{T}} \boldsymbol{\Sigma}^{-1}\left(\boldsymbol{y}_i - \tilde{\mathcal{M}}(\boldsymbol{x})\right)\right)
\end{aligned}$$

Incorporate all uncertainties into Σ

$$\boldsymbol{y} = \tilde{\mathcal{M}}(\boldsymbol{x}) + \overset{\text{Numeric/ Trunction}}{\eta(\boldsymbol{x})} + \overset{\text{Model discrepancy}}{\delta(\boldsymbol{x})} + \overset{\text{Observation error}}{\boldsymbol{\varepsilon}}$$

$$\boldsymbol{\Sigma}$$

Bayesian inference results

Difficulty with calculating evidence $\pi(\mathcal{Y})$

$$\color{red}{\pi(\boldsymbol{x}|\mathcal{Y})} = \frac{\mathcal{L}(\boldsymbol{x}|\mathcal{Y}) \cdot \pi(\boldsymbol{x})}{\pi(\mathcal{Y})}$$

Computing evidence $\pi(\mathcal{Y})$ is not a tractable problem. A common strategy is using *conjugate priors*

- static Bayesian network
- variant elimintion/ belief propagation
- kalman filtering

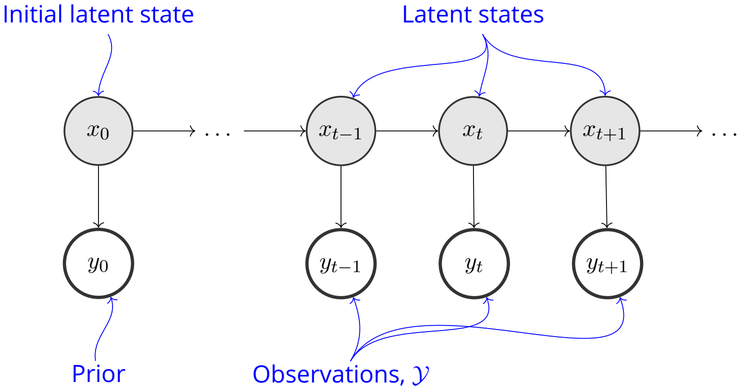
Computational methods:

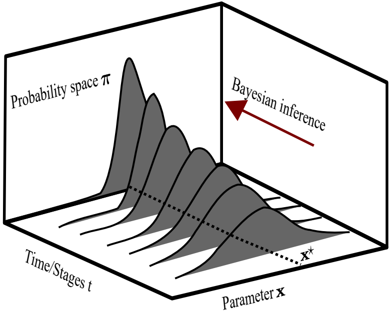
$$\pi(\boldsymbol{x}|\mathcal{Y}) \approx \mathcal{L}(\boldsymbol{x}|\mathcal{Y}) \cdot \pi(\boldsymbol{x})$$

Samples from the posterior can be obtained through *Sampling methods* or *Optimization methods*: *MCMC, variational methods,...*

A unified and scable digital twin

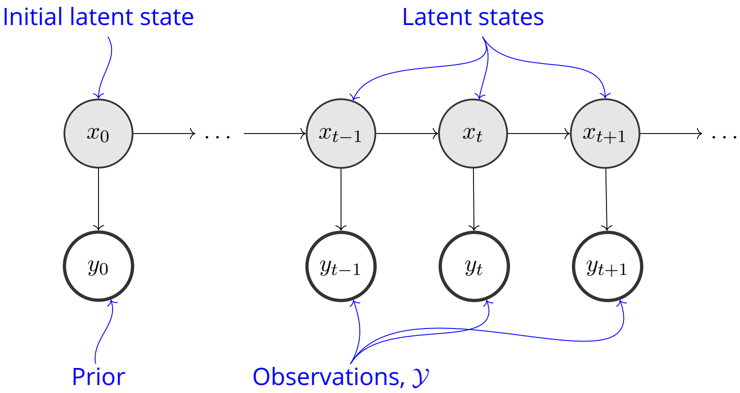
- Visualize the calibration and prediction
- Make prompt actions

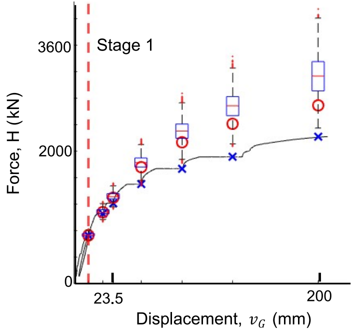




A unified and scable digital twin

- Visualize the calibration and prediction
- Make prompt actions





PISA-Pile CL2

Future considerations:

1. In geotechnical engineering, be careful dealing with aleatoric and epistemic types of uncertainties
2. Four UQ components are equally important.
3. Consider different types of uncertainty into Bayesian inference required linked with likelihood
4. Digital twin-final goal of UQ in geotechnics

References I

- Nagel, Joseph B, Jörg Rieckermann, and Bruno Sudret. "Principal component analysis and sparse polynomial chaos expansions for global sensitivity analysis and model calibration: Application to urban drainage simulation". In: *Reliability Engineering & System Safety* 195 (2020), p. 106737.
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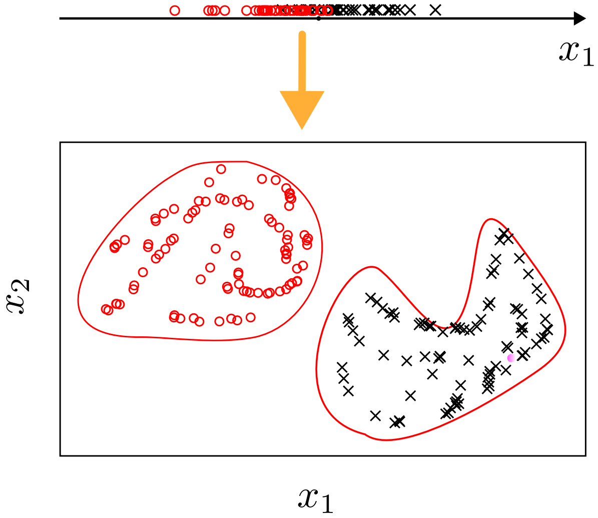
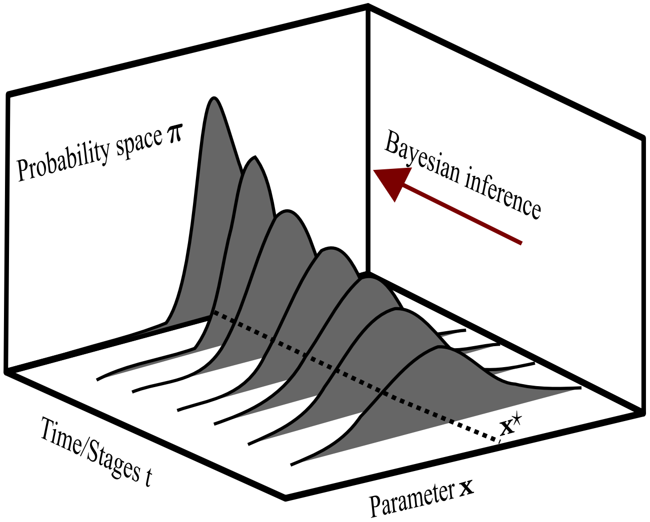
Thank you!

Questions? Comments?

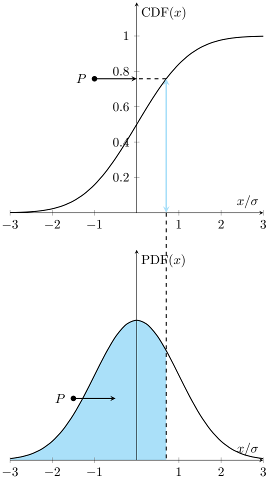
Appendix:

Aleatoric to epistemic

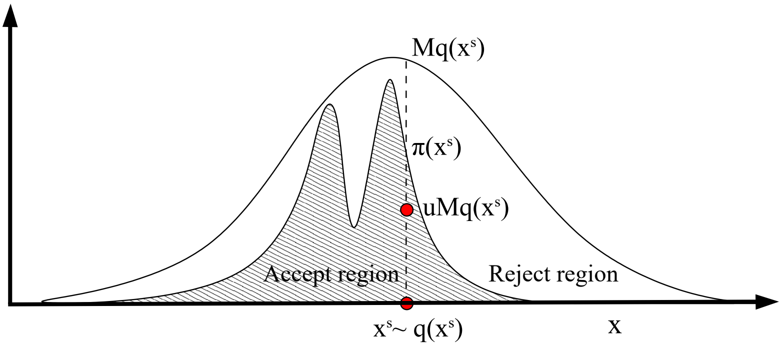



Probability space π
Bayesian inference
Time/Stages t
Parameter $\mathbf{x}$
$\mathbf{x}^{\star}$

- Inverse probability transform



- Rejection sampling



$$E[f(\boldsymbol{x}_t)] = \int f(\boldsymbol{x}_t)\pi(\boldsymbol{x}_t)d\boldsymbol{x}_t \approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}_t^s)$$

$$E[f(\boldsymbol{x}_t)] = \int f(\boldsymbol{x}_t)\pi(\boldsymbol{x}_t)d\boldsymbol{x}_t = \int f(\boldsymbol{x}_t)\frac{\pi(\boldsymbol{x}_t)}{q(\boldsymbol{x}_t)}q(\boldsymbol{x}_t)d\boldsymbol{x}_t \approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}_t^s)\frac{\pi(\boldsymbol{x}_t^s)}{q(\boldsymbol{x}_t^s)}$$

- Require a proper proposal distribution $q(\boldsymbol{x}_t)$

$$f(\boldsymbol{x}_t^{s+1}|\boldsymbol{x}_t^{s}) = \min(1, \alpha)$$

$$\alpha = \min(1, \frac{q(\boldsymbol{x}_t^{s}|\boldsymbol{x}_t^{s+1})\pi(\boldsymbol{x}_t^{s+1}|\mathcal{Y}_t)}{q(\boldsymbol{x}_t^{s+1}|\boldsymbol{x}_t^{s})\pi(\boldsymbol{x}_t^{s}|\mathcal{Y}_t)})$$

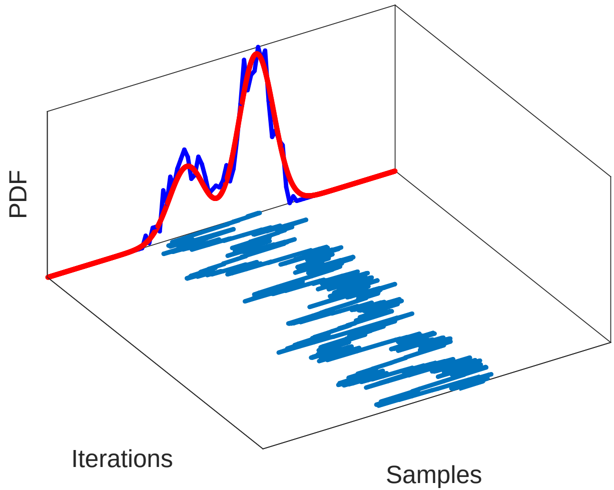
Appendix:

Metropolish-Hasting

Algorithm 1: MH algorithm at t_{th} step

Data: $q(\boldsymbol{x}_t)$: Proposal distribution; $\pi(\boldsymbol{x}_t|\mathcal{Y})$: Target posterior.
Result: MCMC samples at t_{th} stage: $\mathcal{X}_t = \{\boldsymbol{x}_t^1, \cdots, \boldsymbol{x}_t^{N_\mathcal{X}}\}$

Initialization $\boldsymbol{x}_t^1 \in \mathcal{D}_{\boldsymbol{X}}$;
for $s \leftarrow 2$ *to* $N_\mathcal{X}$ **do**
  Sample $\boldsymbol{x}_t^{s+1} \sim q(\boldsymbol{x}_t^{s+1}|\boldsymbol{x}_t^s)$;
  Compute acceptance probability α;
  Compute $f\left(\boldsymbol{x}_t^{s+1}|\boldsymbol{x}_t^s\right) = \min(1, \alpha)$;
  Sample $u \sim \mathcal{U}(0, 1)$;
  Set candidate sample $\boldsymbol{x}_t^{(\star)}$ to $\boldsymbol{x}_t^{s+1}$ with probability α;
end for


PDF
Iterations
Samples

$$\boldsymbol{x}_t^{(\star)} = \boldsymbol{x}_{t\_i}^{(s)} + z \cdot (\boldsymbol{x}_{t\_j}^{(\tilde{s})} - \boldsymbol{x}_{t\_i}^{(s)})$$

$$p(z|a) = \begin{cases} \frac{1}{\sqrt{z}(2\sqrt{a} - \frac{2}{\sqrt{a}})} & \text{if } z \in [1/a, a] \\ 0 & \text{otherwise} \end{cases}$$

$$\alpha = \min(1, z^{M-1} \frac{\pi(x_t^{(\star)}|\mathcal{Y})}{\pi(x_{t\_i}^{(s)}|\mathcal{Y})})$$

Appendix:
AIES

Algorithm 2: AIES algorithm at t_{th} step

Data: $\pi(\boldsymbol{x}_t|\mathcal{Y})$: Target posterior; tuning parameter a

Result: MCMC samples at t_{th} stage: $\mathcal{X}_t = \{\mathcal{X}_{t\_1}, \cdots, \mathcal{X}_{t\_N_{chain}}\}$), with

$$\mathcal{X}_{t\_i} = \{\boldsymbol{x}_{t\_i}^1, \cdots, \boldsymbol{x}_{t\_i}^{N_{\mathcal{X}}}\}$$

```
Initialization N_chain samples {x^1_{t_1}, ..., x^1_{t_N_chain}}, with x^1_{t_i} ∈ D_X
for s ← 2 to N_X do
    for i ∈ {1, ..., N_chain} do
        Pick random j from {1, ..., N_chain}\i;
        Propose x_t^(⋆) with ??;
        Set x^s_{t_i} = x_t^(⋆) with probability α (see ??);
    end for
end for
```

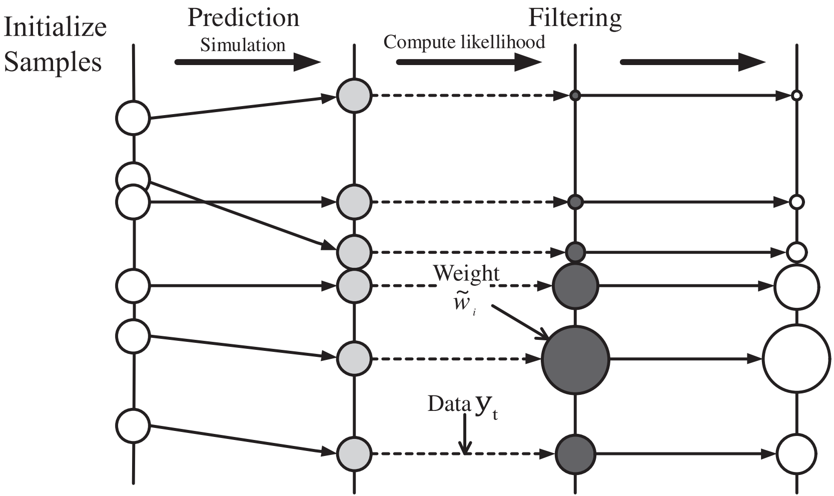
- Initialization N_{chain} samples $\{\boldsymbol{x}_{t\_1}^1, \cdots, \boldsymbol{x}_{t\_N_{chain}}^1\}$, with $\boldsymbol{x}_{t\_i}^1 \in \mathcal{D}_{\boldsymbol{X}}$
- **for** $s \leftarrow 2$ *to* $N_{\mathcal{X}}$ **do**
  - **for** $i \in \{1, \cdots, N_{chain}\}$ **do**
    - Pick random j from $\{1, \cdots, N_{chain}\}\backslash i$;
    - Propose $x_t^{(\star)}$ with **??**;
    - Set $\boldsymbol{x}_{t\_i}^s = x_t^{(\star)}$ with probability α (see **??**);
  - **end for**
- **end for**

$$\boldsymbol{x_t} = g(\boldsymbol{x_{t-1}}) + \boldsymbol{v} \qquad \text{(state equation)}$$
$$\mathcal{Y}_t = m(\boldsymbol{x_t}) + \boldsymbol{w} \qquad \text{(observation equation)}$$

$$\pi(\boldsymbol{x}_{1:t}|\mathcal{Y}_{1:t}) \approx \sum_{s=1}^{S} \tilde{w}_t^s \delta_{\boldsymbol{x}_{1:t}^s}(\boldsymbol{x}_{1:t})$$

$$\tilde{w}_t^s = \frac{w_t^s}{\sum_{s=1}^{S}(w_t^s)}$$

$$\pi(\boldsymbol{x}_{1:t}|\mathcal{Y}_{1:t}) \propto \pi(\mathcal{Y}_t|\boldsymbol{x}_t)\pi(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})\pi(\boldsymbol{x}_{t-1}|\mathcal{Y}_{t-1})$$



Initialize Samples
Prediction
Simulation
Filtering
Compute likellihood
Weight
$\tilde{w}_i$
Data y_t

Appendix:

Sequential Monte Carlo with resampling

Algorithm 3: SISR algorithm at t_{th} step

Data: Samples $\boldsymbol{x}_{t-1}^s$ with weights w_{t-1}^s, $s = \{1, \cdots, N\}$; observation $\mathcal{Y}_t$ at t_{th} stage

Result: SMC samples with normalized weights $\tilde{w}_t^s$ at t_{th} stage: $\boldsymbol{x}_t^{(\star)} = \{\boldsymbol{x}_t^1, \cdots, \boldsymbol{x}_t^N\}$)

for $s \leftarrow 1$ *to* N **do**

  Sample from proposal distribution $\boldsymbol{x}_t^s \sim q(\boldsymbol{x}_t^s | \boldsymbol{x}_{t-1}^s, \mathcal{Y}_t)$;

  Compute weight using **??**;

end for

Normalized weights;

Calculate degeneracy measure using **??**;

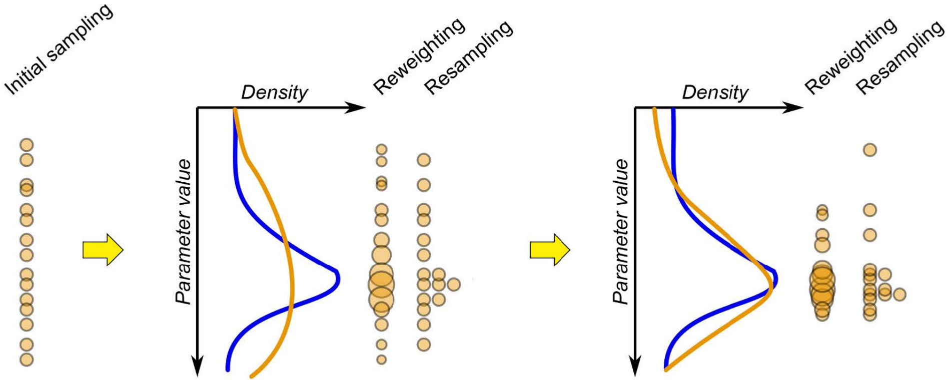
if $\hat{S}_{eff} < S$ **then**

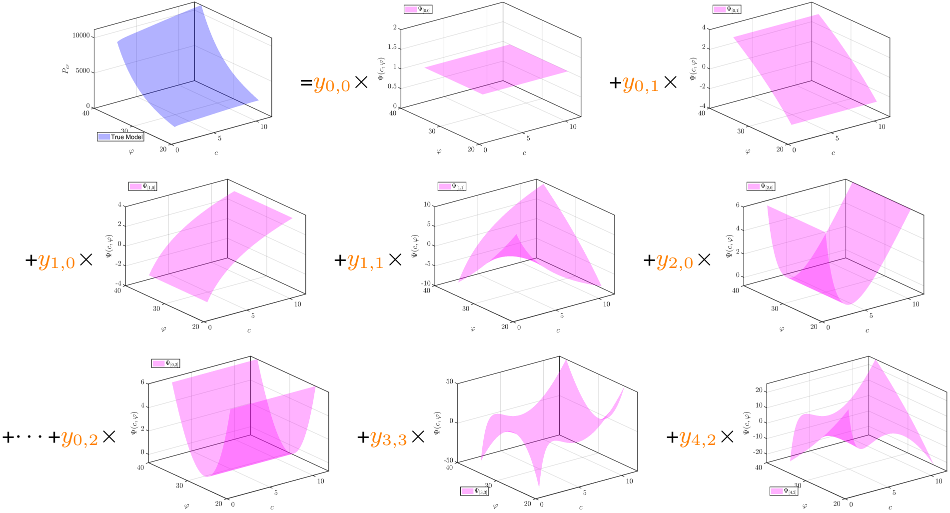
  Resample;

end if

Appendix:

Sequential Monte Carlo with resampling





$$= y_{0,0} \times \quad + y_{0,1} \times \quad + y_{1,0} \times \quad + y_{1,1} \times \quad + y_{2,0} \times \quad + \cdots + y_{0,2} \times \quad + y_{3,3} \times \quad + y_{4,2} \times$$