Uncertainty quantification (UQ) in geotechnical engineering

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Presentation Overview

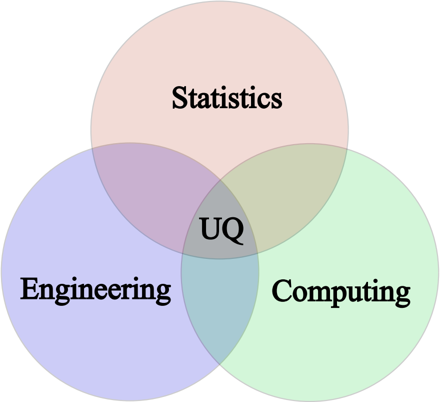
What is Uncertainty Quantification (UQ)?

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

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

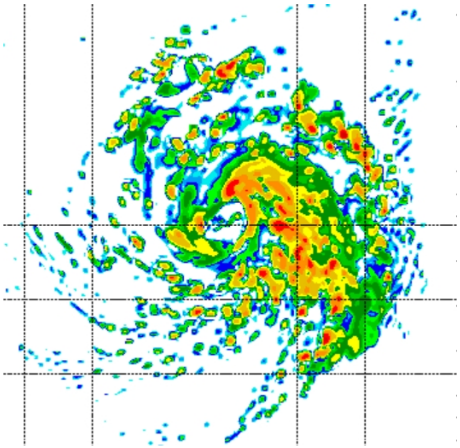
UQ provides a framework for answering these question and making models useful.

What is Uncertainty Quantification (UQ)?



Uncertainty quantification (UQ) is the science of quantitative characterization and estimation of uncertainties in both computational and real world applications. It tries to determine how likely certain outcomes are if some aspects of the system are not exactly known. . . –Wikipedia

Real world with uncertainties



Source: Wikipedia

Types of two uncertainties

Aleatoric vs epistemic

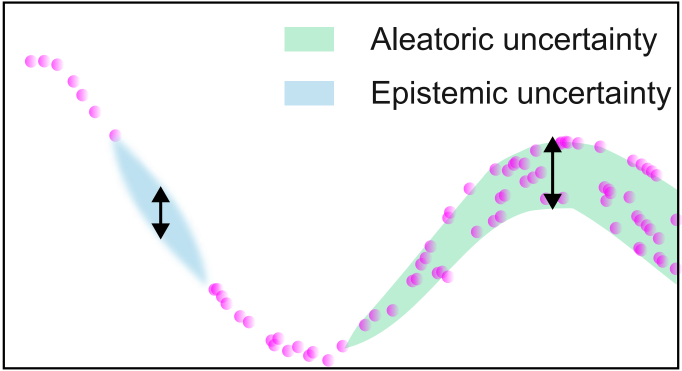


Figure: Aleatoric uncertainty vs Epistemic uncertainty

Distinguish:

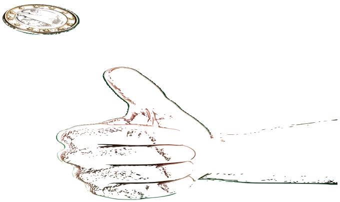
Aleatoric uncertainty

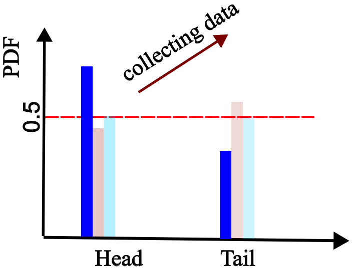
statistical variability, inherently random effects (**irreducible**)

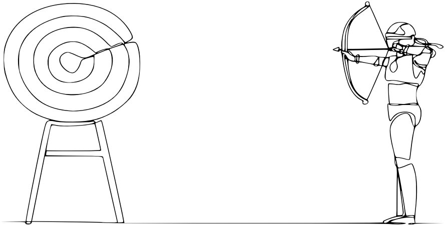
Epistemic uncertainty

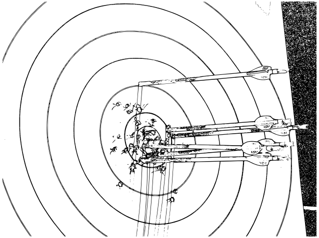
model uncertainty, a lack of knowledge (**reducible**)

Type one: aleatoric uncertainty

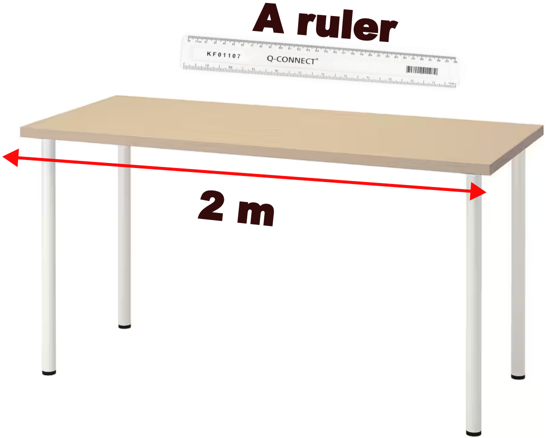








Type two: epistemic uncertainty



Random variables:

$x_i = x^{\star}(\text{2m}) \pm \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma^2)$

$x_i \sim iid$

$\boldsymbol{x} = (x_1, x_2, \cdots, x_n)$

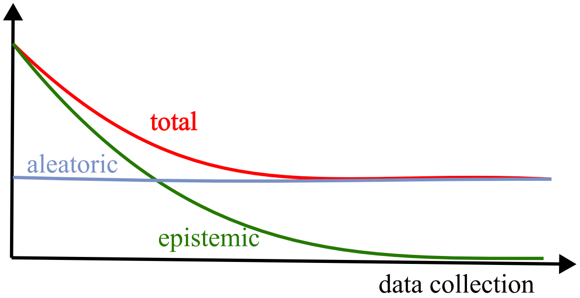
mean:

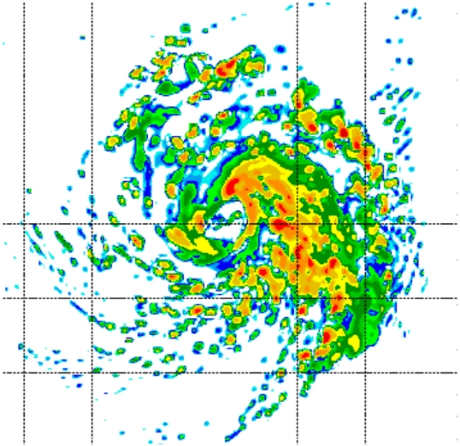
$$\begin{aligned} \mathbb{E}(\boldsymbol{x}) &= \frac{1}{n}\sum_{i=1}^{n} x_i \\ &= \mathbb{E}(x^{\star})(\text{2m}) + \mathbb{E}(\boldsymbol{\epsilon}) \end{aligned} \quad (1)$$

When $n \to \infty$, $\mathbb{E}(\boldsymbol{x}) \approx x^{\star} + 0 \approx$ 2 (m)

Uncertainty components:

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

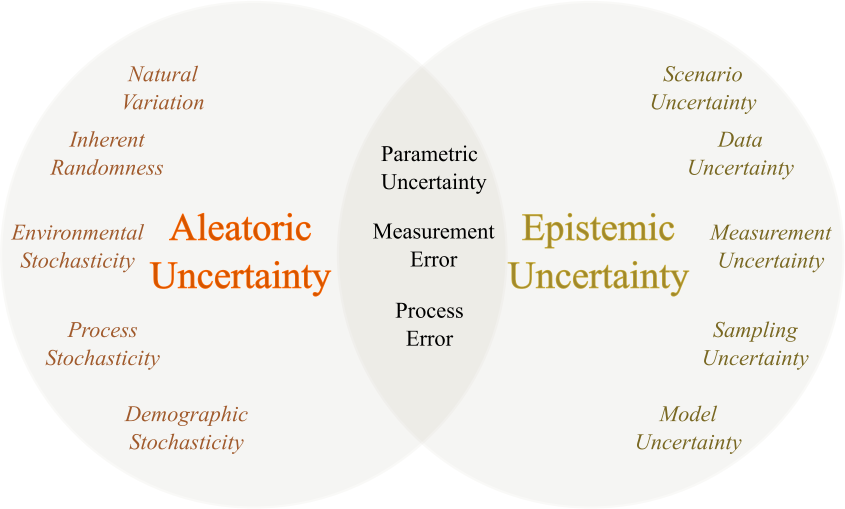




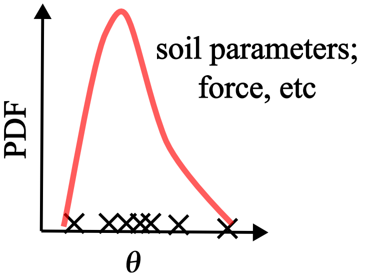
Source: Wikipedia

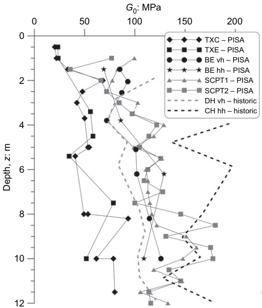
Not simple as it is

Mix of aleatoric and epistemic: Involve too much subjectivity



What about uncertainties in geotechnics





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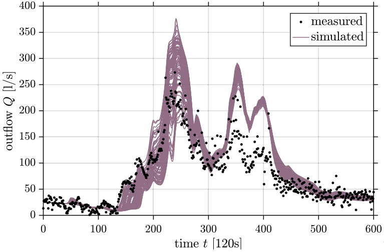

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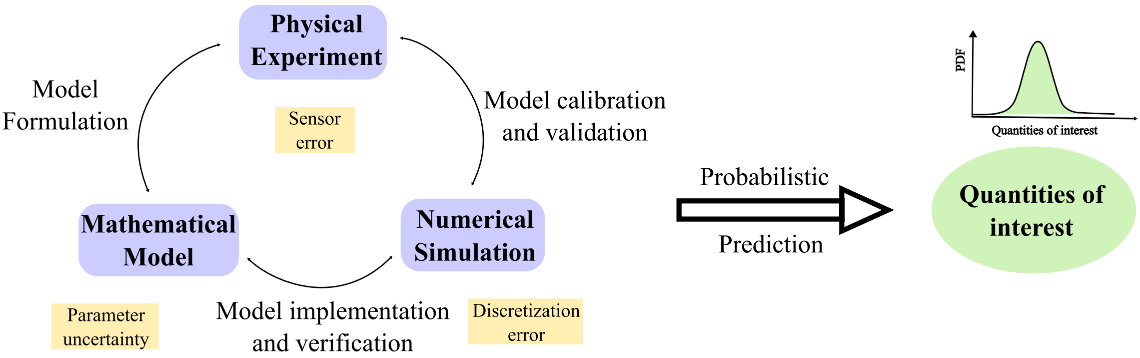
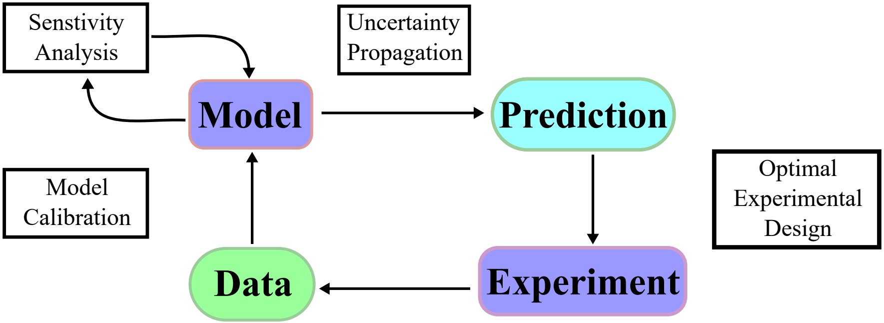
[1] Lidija Zdravković et al. "Ground characterisation for PISA pile testing and analysis". In: *Géotechnique* 70.11 (2020), pp. 945–960.

[2] 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.

Experiments, Models, Simulations, and UQ

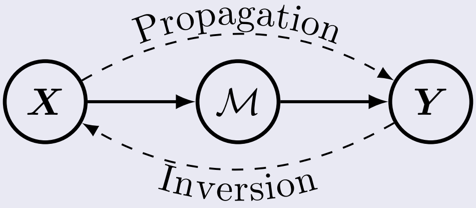


UQ problems and components



UQ problems and components

Two UQ types of problems:



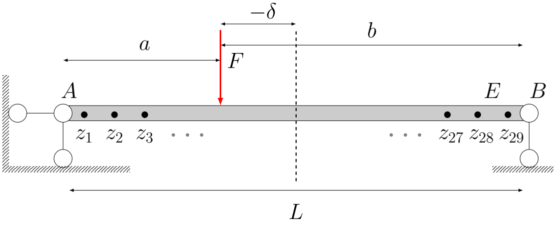
Four components:

1. Uncertainty propagation
2. Model calibration
3. Sensitivity analysis
4. Optimal experimental design

Definition

A computational model should contain:

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



$$y = \begin{cases} \frac{Fbx[(L^2-b^2)-x^2]}{6LEI} & x \leq a \\ \frac{Fb[\frac{L}{b}(x-a)^3+(L^2-b^2)]}{6LEI} & x > a \end{cases} \tag{2}$$

Definition

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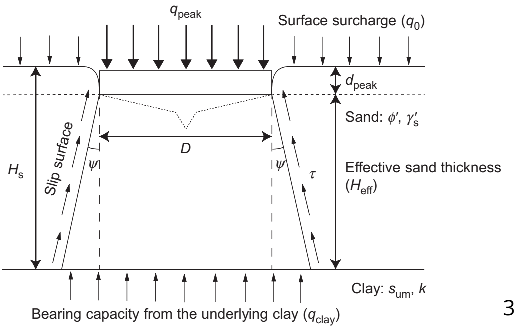

[3]

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Definition

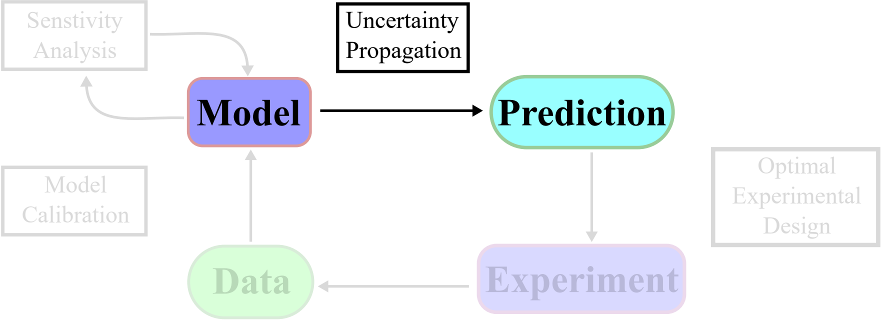
A computational model should contain:

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

Numerical methods:

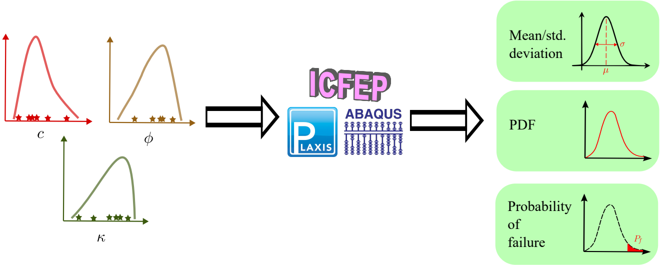
- Finite element method
- Finite difference method
- . . .

UQ components one-Uncertainty propagation



- Uncertainty propagation feeds quantified input uncertainties through our model to produce probabilistic predictions of a QoI

UQ components one-Uncertainty propagation



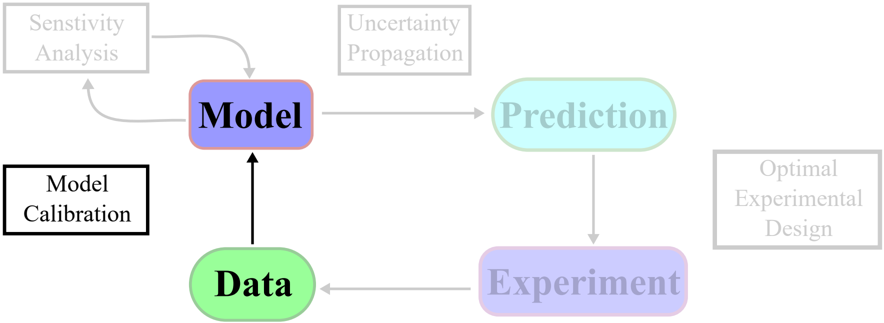
- Output statistics, i.e., mean, standard deviation. etc.

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

- Distribution of the QoI

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

UQ components two-Model calibration



- Model calibration explicitly quantifies model input uncertainties using experimental data (improve/update initial assumptions)

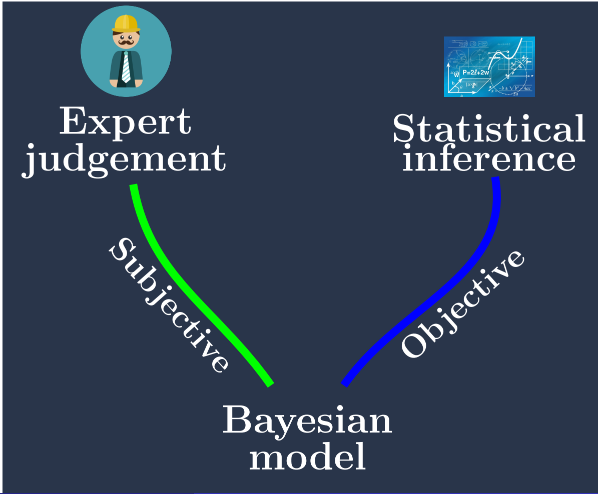
UQ components two-Model calibration

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

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

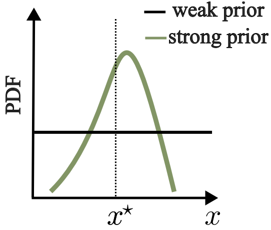


UQ components two-Model calibration

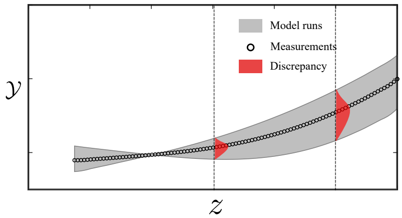
Bayesian methods

Expert guess + Limited data $\rightarrow$ Distribution

Prior:



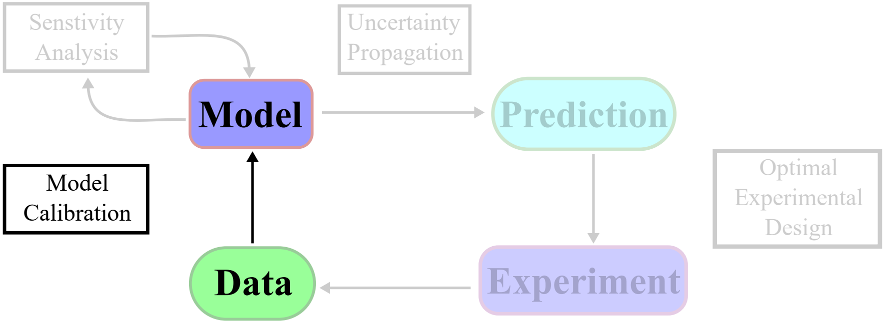
Likelihood:



Notable caveats:

- Prior-Requires specific expertise
- Likelihood-Computationally expensive

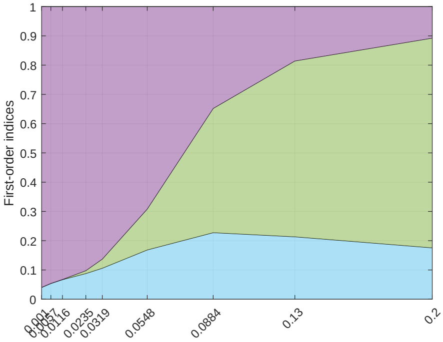
UQ components three-Sensitivity analysis



- Sensitivity analysis identifies the most influential parameters

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 paramters



UQ components three-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:

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

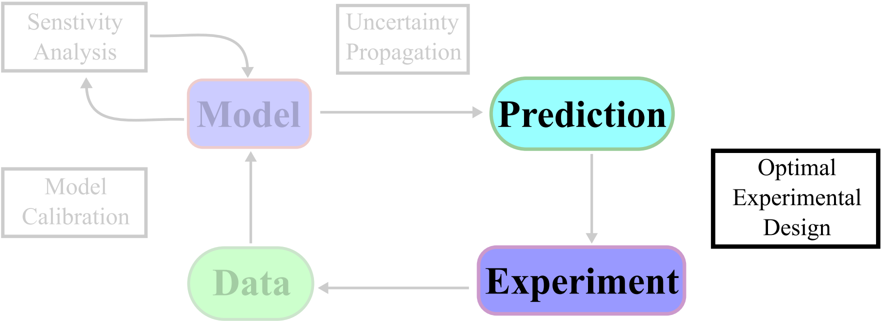
  Quantify the effect of each input parameter separately

- Total Sobol's indice:

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

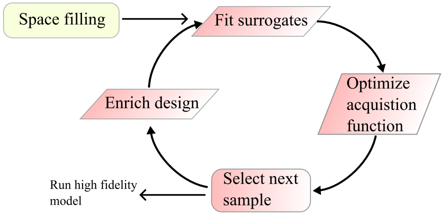
  Quantify the total effect of x_i, including interactions with other variables

UQ components three-Optimum Experimental design



UQ components three-Optimum Experimental design

Surrogate model	Reliability estimation	Learning function	Stopping criteria
Kriging	Monte Carlo	EFF	Bounds on P_f
PCE	Subset simulation	FBR	...
SVR	Importance sampling	...	
PCK	...		
Physics-based types			
...			



- Not each run is equally important
- Save time

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
- ...

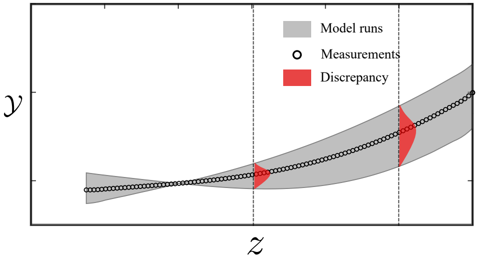
Connecting physics with FE modelling

Through an additive observation error:

$$\boldsymbol{y} = \mathcal{M}(\boldsymbol{x}) + \varepsilon \tag{2}$$

The rationale behind the equation:

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



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

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

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 $\pi(\mathcal{Y})$

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

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

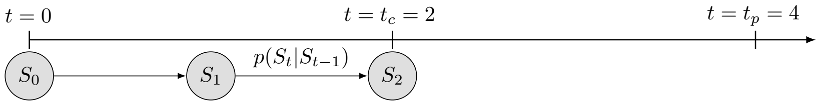
Computational methods:

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

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

A unified and scalable digital twin

- Visualize the sequential inversion calculation
- Bring in control theory naturally to make prompt actions
- Support the transition from custom defined model towards a unified and scalable digital twin



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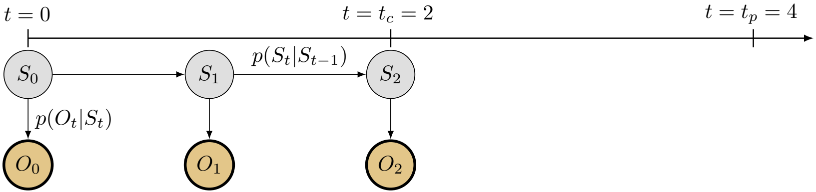

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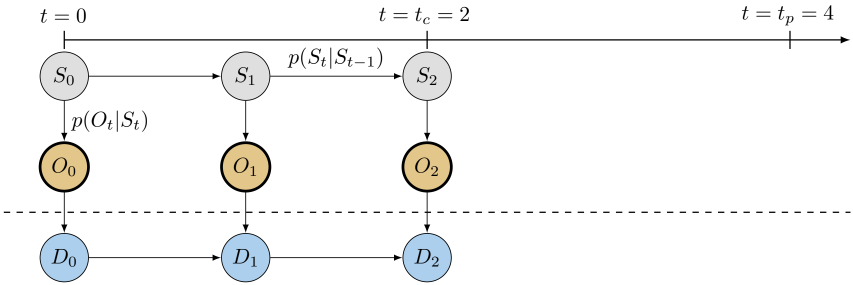

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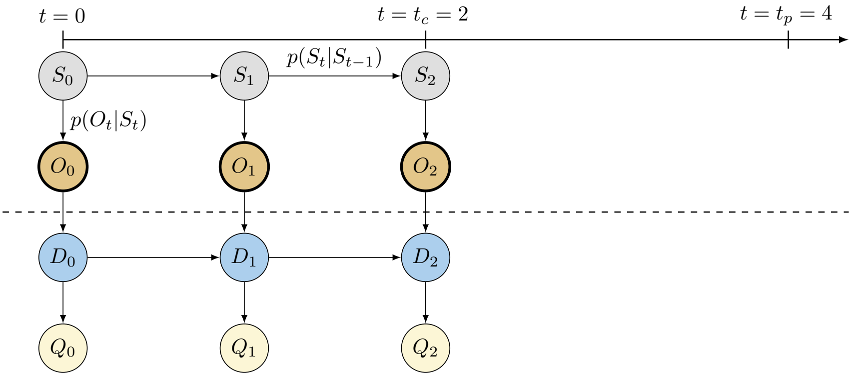

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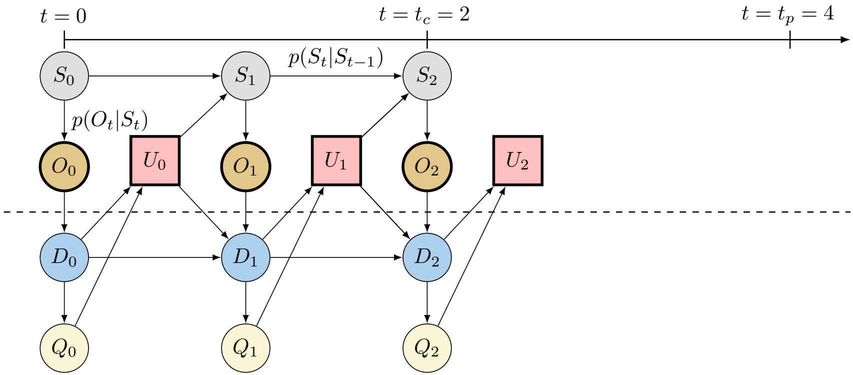

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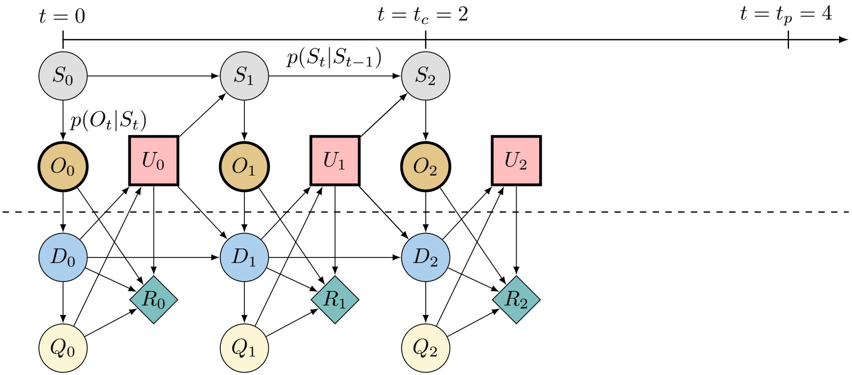

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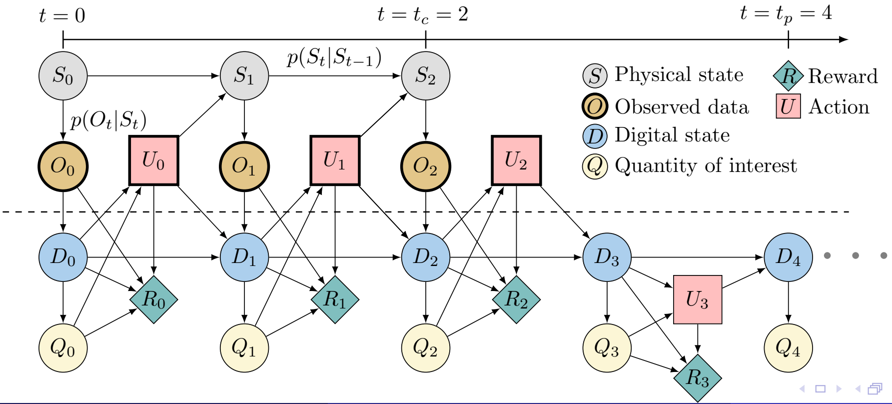

Conclusion

1. In engineering, we should notice which uncertainty is aleatoric or epistemic or mixed type
2. Aleatoric uncertainty should be considered even it is irreducible
3. Four UQ components are equally important
4. Consider different types of uncertainty into Bayesian inference required linked with likelihood
5. Digital twin-final goal of UQ in geotechnics

References I

- Li, Jinhui et al. "Bayesian prediction of peak resistance of a spudcan penetrating sand-over-clay". In: *Géotechnique* 68.10 (2018), pp. 905–917.
- 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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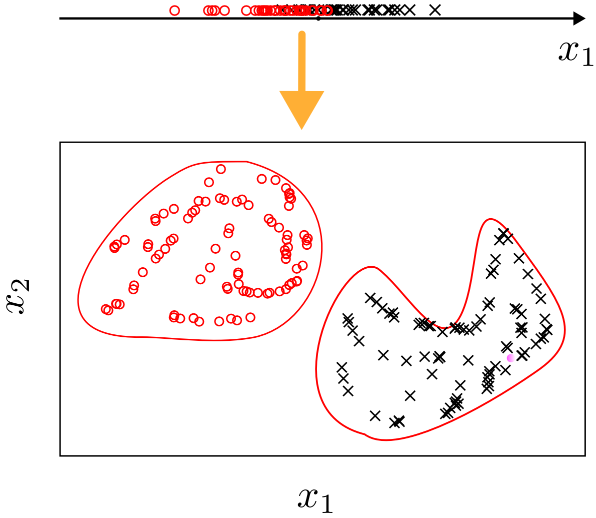
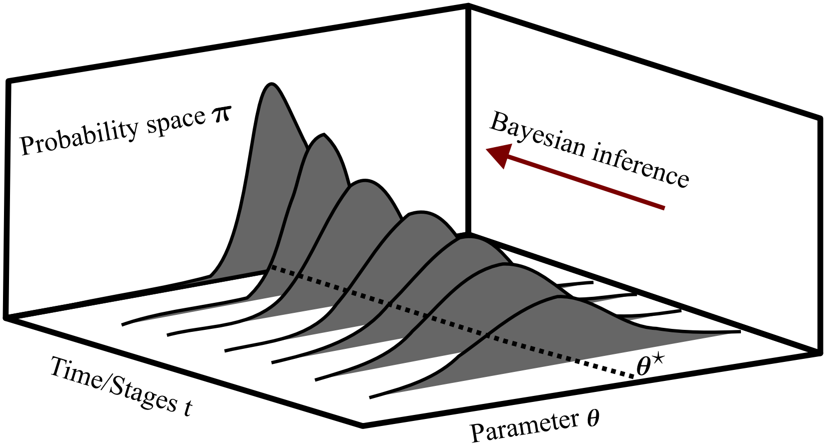
Thank you!

Questions? Comments?

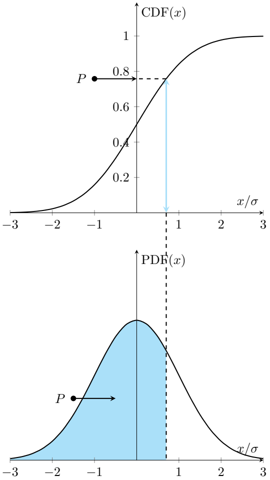


x_1
x_2
x_1

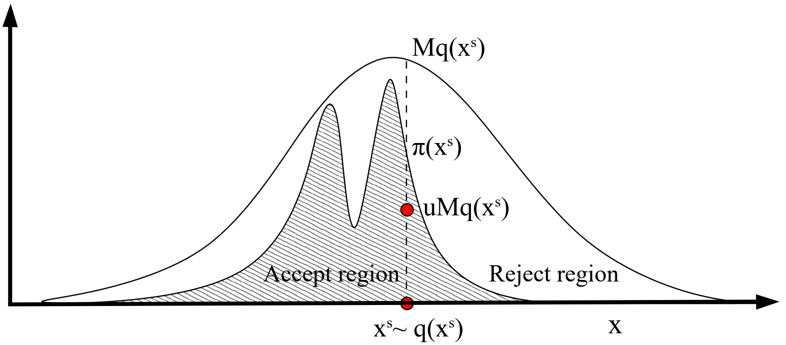


Probability space π
Bayesian inference
$\theta^\star$
Time/Stages t
Parameter θ

- Inverse probability transform



- Rejection sampling



Appendix:

importance 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: $\mathcal{X}_t = \{\boldsymbol{x}_t^1, \cdots, \boldsymbol{x}_t^{N_\mathcal{X}}\}$

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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 $\alpha$;
    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 $\alpha$;
end for
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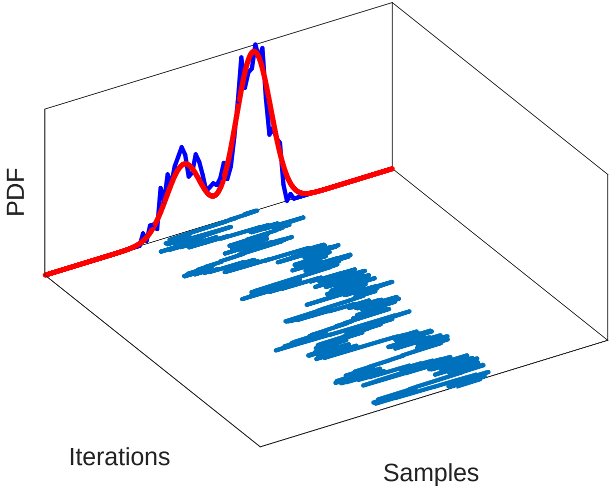


PDF
Iterations
Samples

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

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

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

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

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

Initialization N_{chain} samples $\{\boldsymbol{x}^1_{t\_1}, \cdots, \boldsymbol{x}^1_{t\_N_{chain}}\}$, with $\boldsymbol{x}^1_{t\_i} \in \mathcal{D}_{\boldsymbol{X}}$

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 $x^{(\star)}_t$ with **??**;

    Set $\boldsymbol{x}^s_{t\_i} = x^{(\star)}_t$ with probability α (see **??**);

  end for

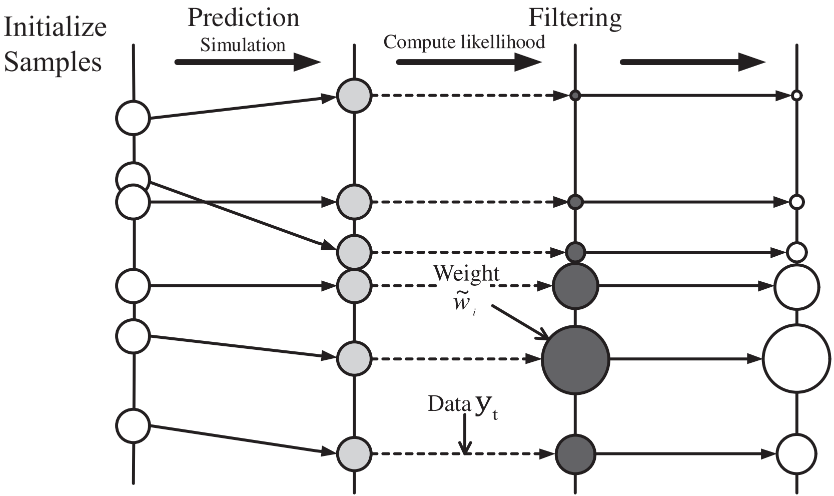
end for

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

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

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

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



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: $\boldsymbol{x}_t^{(\star)} = \{\boldsymbol{x}_t^1, \cdots, \boldsymbol{x}_t^N\}$)

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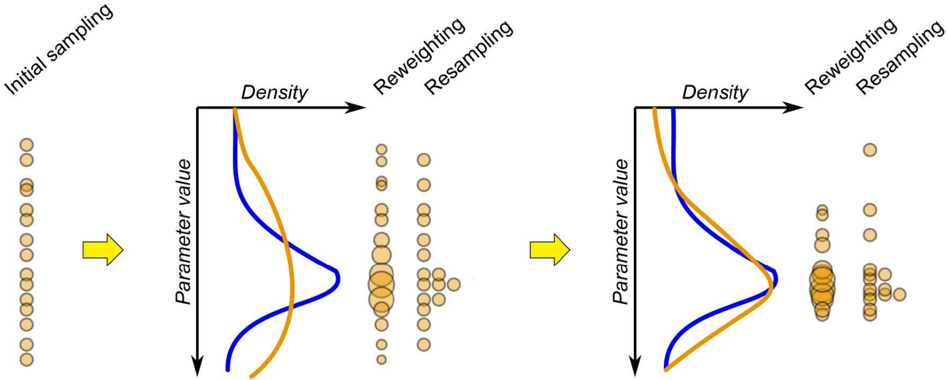
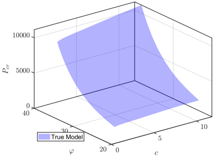
for s ← 1 to N do
    Sample from proposal distribution x_t^s ~ q(x_t^s | x_{t-1}^s, Y_t);
    Compute weight using ??;
end for
Normalized weights;
Calculate degeneracy measure using ??;
if Ŝ_eff < S then
    Resample;
end if
```

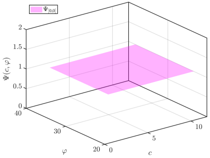
Appendix:

Sequential Monte Carlo with resampling

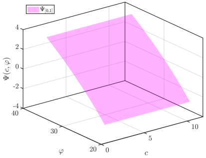




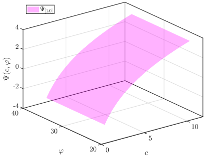
$= y_{0,0} \times$



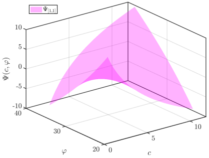
$+ y_{0,1} \times$



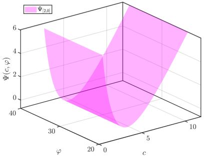
$+ y_{1,0} \times$



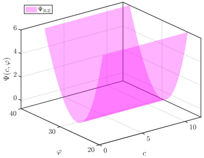
$+ y_{1,1} \times$



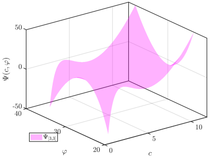
$+ y_{2,0} \times$



$+ \cdots + y_{0,2} \times$



$+ y_{3,3} \times$



$+ y_{4,2} \times$