Bayesian Calibration of Multi-Physics Models

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Motivation

• Uncertainty quantification in model parameters: infer/calibrate the probability distributions of parameters from available data

Bayes Network

- A probabilistic graphical model that represents a set of random variables and their conditional dependencies via a directed acyclic graph
- Can include various sources of uncertainty, errors, model predictions and experimental data
- Systematic way to combine multiple sources of uncertainty



Example

• Bayes network for two physics models \rightarrow pull-in voltage model and creep model • Data of pull-in voltage for Device 1, and data of creep deflection for Device 2 are available • Device 1 and 2 are made of the same material (i.e., the same Young's modulus E)



f(U) = f(a)f(b|a) $f(c \mid a)$ $f(d \mid c)$ f(e|b,d)f(f)f(g|e,f)



Figure 1: Concept of Bayes Network

Model Calibration with Bayes Network

• Computational model $y = G(x; \theta)$

$$\begin{array}{cccc} \text{Input } x \longrightarrow & \text{Model } G & \longrightarrow & \text{Output } y \longrightarrow & \text{Data } y_D \\ & & \uparrow & & & \uparrow \\ & \text{Parameter } \theta & & \text{Model form error } \varepsilon_{mf} (\text{unknown}) \\ & \text{Measurement noise } \varepsilon_{obs} \sim N(0, \sigma_{obs}) \end{array}$$

$$\bullet \text{ Bayesian calibration } & \pi(\theta \mid y_D) = \frac{\Pr(y_D \mid \theta) \pi(\theta)}{\int \Pr(y_D \mid \theta) \pi(\theta) d\theta} \end{array}$$

- \succ Pr($y_D | \theta$) : likelihood function of θ (derived from the conditional probabilities in the Bayes network)
- prior probability density function of θ $\succ \pi(\theta)$:
- $\succ \pi(\theta|y_D)$: updated probability density function of θ

• Option 1. Calibration with information flowing from sub-network (A) to (B)

• (1.1) Calibration of the pull-in voltage model

> Calibrate model parameters (*E* and σ_{rs}) and ε_{mf1} (assumed as a random variable) together



• (1.2) Calibration of the creep model

 \succ Calibrate the creep model, with the posterior PDF of E obtained in (1.1) as the prior of E



Imprecise (Interval) Experimental Data

• The voltage is increased in 5-volt steps during the measurement

 \rightarrow pull-in voltage is reported within a 5-volt range \rightarrow interval data Incorporate interval data into likelihood function

$$\Pr(y_D \mid \theta) = \Pr(y_D^1 \le y_D \le y_D^2) = \int_{y_D^1}^{y_D^2} \pi(y_D \mid \theta) dy_D$$

Time series data

• Creep deflection is measured at multiple time points \rightarrow time series data Incorporate time series data into likelihood function

 $\Pr(\mathbf{y}_{\mathbf{D}}^{\mathbf{t}} \mid \boldsymbol{\theta}) \propto (2\pi)^{-n/2} \mid \boldsymbol{\Sigma} \mid^{-1/2} \exp[-\frac{1}{2}(\mathbf{y}_{\mathbf{D}}^{\mathbf{t}} - \boldsymbol{\mu}_{t})\boldsymbol{\Sigma}^{-1}(\mathbf{y}_{\mathbf{D}}^{\mathbf{t}} - \boldsymbol{\mu}_{t})^{T}]$

Note: If model output y_t is a Gaussian vector with mean μ_t and covariance matrix Σ_{v} , $\mathbf{y}_{\mathbf{D}}^{t}$ is also a random vector with mean μ_{t} and covariance matrix $\Sigma = \Sigma_{v} + 1$ σ^{2}_{obs}

Quantification of Model Form Error

• Two possible methods

(1) Calibrate ε_{mf} and model parameters together \rightarrow increases the dimension

• Option 2. Calibration with information flowing from sub-network (B) to (A)

• (2.1) Calibration of the creep model

> Calibrate model parameters (A_c and E) and ε_{mf2} (assumed as a random variable) together



• (2.2) <u>Calibration of the pull-in voltage model</u>

205

0.02

190

195 *E* (GPa)

200

 \succ Calibrate the pull-in voltage model, with the posterior PDF of E obtained in (2.1) as the prior of E

0.01

50

40

-20

-30

-10

0

 $\varepsilon_{mf1}(\text{volt})$

10

20 30



 $\sigma_{rs}(MPa)$

30

of calibration variables (more feasible if ε_{mf} is treated as a random variable)

(2) Calibrate model parameters first, and then estimate ε_{mf} by comparing

updated model and data \rightarrow computationally efficient even when ε_{mf} is

treated as a random process indexed by the model input *x*

Note: Both options of calibration give the same updated PDF of *E*

10

0.02

-10

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