Computer model calibration for design, with an application to wind turbine blades

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Computer experiments

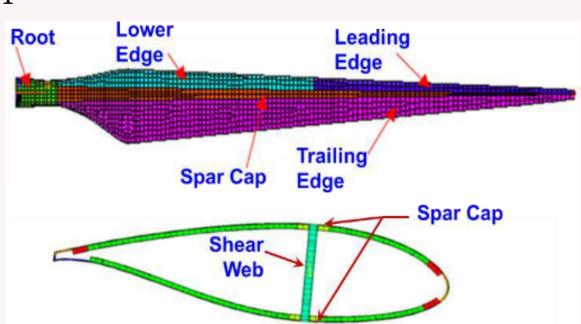
Researchers increasingly look to computer experiments to investigate phenomena where physical experimentation is difficult or impossible[1].

Computer model calibration

- Computer models may include unknown inputs (calibration inputs) which must be estimated.
- E.g.: a model's output depends upon a physical constant which is unknown.
- Calibration input is often estimated by combining simulator output with field data.
- Calibration is ordinarily thought of as bringing a computer model into agreement with reality.

Finite element smulator

We rely on a finite element simulator of the blade cost and performance.



- Calibration inputs are volume fraction and thickness of the blade material.
- Control input is temperature.
- Outputs are tip deflection, rotation, and cost; the design goal is to minimize these.
- Model utilizes ANSYS simulation software.
- ANSYS model cost too high for use in MCMC.

References

[1] Jerome Sacks, William J. Welch, Toby J. Mitchell, and Henry P. Wynn. Design and Analysis of Computer Experiments.

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Central idea

Previous explorations of computer model calibration have approached calibration as a matter of bringing a computer model into agreement with physical reality. In the present work, we consider computer model calibration as a method for design. Under this framework, we calibrate a computer model not using physical experimental data, but rather using "desired data" which describes the performance one hopes to achieve in the simulated system.

Gaussian process emulator

Gaussian processes (GPs) can be thought of as random functions, which are generalizations of multivariate normal random variables. A GP is fully characterized by its mean function $\mu: D \to R$ and covariance function $V: D \times D \to R$, where D is the domain of the process.

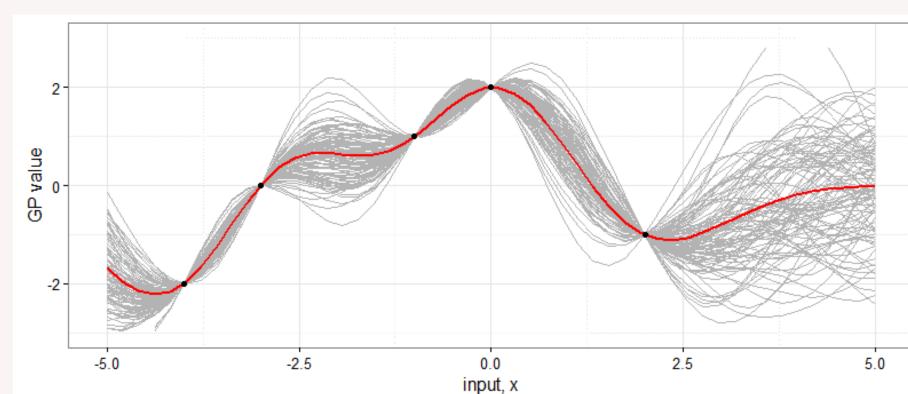


Figure 1:Example of a univariate Gaussian process

GPs are advantageous for emulating computationally expensive deterministic computer code because

- Use of a GP does not require detailed foreknowledge of the approximate parametric form of the model; we often lack such knowledge
- GPs easily interpolate the observed data; since the simulation code is deterministic and free of observation error, this is desirable
- The variance of GPs provides a natural form of uncertainty quantification (see Figure 1)

Emulator implementation

Model inputs are a dummy input x_1 (to convert trivariate output into univariate), temperature x_2 , volume fraction x_3 and thickness x_4 . For our GP emulator prior we use the covariance function

$$V(\mathbf{x}, \mathbf{x}') = \frac{1}{\lambda} \exp\{-\sum_{i=1}^{4} \beta_i (x_i - x_i')^2\}$$

where λ , β were estimated using gradient methods to find their MLEs. A prior mean $\mu(\mathbf{x}) = 0$ was also used. Observations $\eta(\mathbf{x}_i)$, $i = 1, \dots, 504$ were collected from the simulation model using a LHC design. The updated (posterior) GP emulator has mean given by

$$\mu^*(\mathbf{x}) = v(\mathbf{x})^T \Sigma^{-1} \boldsymbol{\eta}$$

where $v(\mathbf{x}) = (V(\mathbf{x}, \mathbf{x}_1), \dots, V(\mathbf{x}, \mathbf{x}_{504}))^T$, Σ is a matrix with $\Sigma_{i,j} = V(\mathbf{x}_i, \mathbf{x}_j)$, and $\boldsymbol{\eta} = (\eta(\mathbf{x}_1), \dots, \eta(\mathbf{x}_{504}))^T$. The updated covariance:

$$V^*(\mathbf{x}, \mathbf{x}') = V(\mathbf{x}, \mathbf{x}') - v(\mathbf{x})^T \Sigma^{-1} v(\mathbf{x}')$$

Desired data

We calibrate the model to "desired data" which reflect extremely low tip deflection, rotation, and cost. Because we are antecedently ignorant of how close the model can come to our desired data, we place an improper $1/\sigma^2$ prior on the observation variance of each model output. We considered a range of desired outcomes.

Full model

Where $\boldsymbol{\theta}$ is the vector of true (optimal) values of the calibration parameter, \mathbf{w} is a vector of control parameter settings, and $\boldsymbol{\epsilon} \sim N_3(0, \operatorname{diag}(\sigma_d^2, \sigma_r^2, \sigma_c^2))$, we may describe the model for the desired data as

$$f(\mathbf{w}, \boldsymbol{\theta}) = f(\mathbf{w}) = f(\eta(\mathbf{w}, \boldsymbol{\theta}) + \boldsymbol{\epsilon})$$

MCMC implementation

- Calibrate volume fraction and thickness to the desired data. Set a uniform prior over each.
- Each iteration of the MCMC, draw new values for x_3, x_4 , and the observation variances.
- Where \mathbf{y} is the desired data, $\mathcal{D} = (\mathbf{y}, \boldsymbol{\eta})^T$ and $\Sigma_{\mathcal{D}} = \operatorname{Var}(\mathcal{D})$, the likelihood of \mathcal{D} is

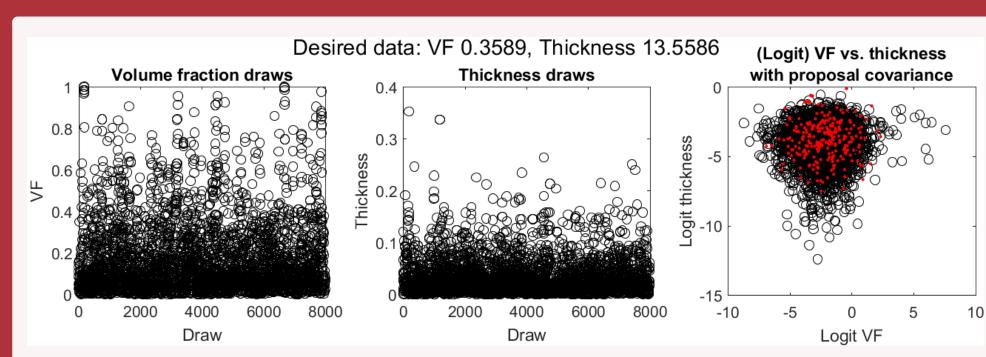
$$L(\mathcal{D}|x_3, x_4, \lambda, \boldsymbol{\beta}, \Sigma_{\mathcal{D}}) = |\Sigma_{\mathcal{D}}|^{-\frac{1}{2}} \exp\{-\frac{1}{2}\mathcal{D}^T \Sigma_{\mathcal{D}}^{-1} \mathcal{D}\}$$

hence the full posterior density is

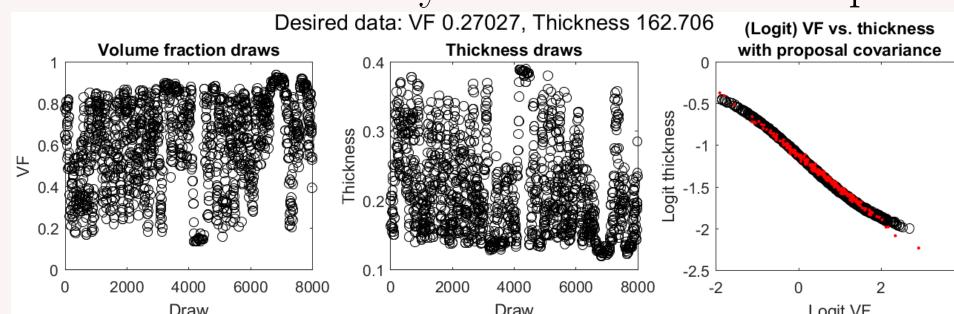
$$\pi(x_3, x_4, \sigma_d^2, \sigma_r^2, \sigma_c^2) \propto \frac{L(\mathcal{D}|x_3, x_4, \lambda, \boldsymbol{\beta}, \Sigma_{\mathcal{D}})}{\sigma_d^2 \sigma_r^2 \sigma_c^2}$$

- Eliminate boundary constraints: $z_i = \text{logit}(x_i)$, $\tau_j = \log(\sigma_i^2)$ for i = 3, 4, j = d, r, c.
- Use Metropolis-Hastings algorithm; normal proposals on $z_i^{(n)}|z_i^{(n-1)}$ and $\tau_j^{(n)}|\tau_j^{(n-1)}$, $\forall i \forall j$.
- In burn-in, the proposal distribution adapts using the sample covariance of previous draws, achieving optimal acceptance ratios ($\sim 40\%$).

Results



- Posterior means are sensitive to choice of desired data. Therefore it is advisable to consider a surface over a range of desired data.
- Where desired output is insufficiently ambitious, the MCMC output reflects this as a lack of identifiability in the calibration inputs.



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