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

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Computer model calibration

- Computer models may include unknown inputs that must be estimated[1]. These inputs are often estimated by combining simulator output with field data.
- Calibration is ordinarily thought of as bringing a computer model into agreement with reality.

Full model

- Where f is the true system, η the computer model of f, δ the discrepancy $f - \eta$, $\boldsymbol{\theta}$ the true values of the calibration parameters, $\mathbf{x}$ the control inputs, and $\boldsymbol{\epsilon}$ error, we have $f(\mathbf{x}, \boldsymbol{\theta}) \equiv f(\mathbf{x}) = \eta(\mathbf{x}, \boldsymbol{\theta}) + \delta(\mathbf{x}) + \boldsymbol{\epsilon}$.
- When η is computationally expensive, we use a mean-zero Gaussian process (GP) emulator as a code surrogate. δ is also modeled using a mean-zero GP. Both GPs use a power product exponential covariance function: respectively (where $\mathbf{x} \in \mathbb{R}^p$, $\boldsymbol{\theta} \in \mathbb{R}^q$),

$$C_\eta((\mathbf{x},\boldsymbol{\theta}),(\mathbf{x}',\boldsymbol{\theta}')) = \frac{1}{\lambda_\eta} \prod_{k=1}^{p} (\rho_k^\eta)^{(x_k - x_k')^2} \times \prod_{j=1}^{q} \left(\rho_{p+j}^\eta\right)^{(\theta_j - \theta_j')^2},$$

$$C_\delta(\mathbf{x}, \mathbf{x}') = \frac{1}{\lambda_\delta} \prod_{k=1}^{p} \left(\rho_k^\delta\right)^{(x_k - x_k')^2}$$

We use the MLEs of λ_η and $\boldsymbol{\rho}^\eta$, set $\rho_i^\delta \sim \text{Beta}(1, 0.3)$ for all i, and set an informative Gamma prior on λ_δ based on what is known *a priori* about the system optimum.

- Let $\boldsymbol{\eta}$ be a vector of univariate observations of the computer model at points $\{(\mathbf{x}_i, \boldsymbol{\theta}_i)\}_{i=1}^{m}$ and $\mathbf{y}$ be a set of "desired observations" at points $\{(\mathbf{x}_i, \boldsymbol{\theta}_i)\}_{i=m+1}^{m+n}$. Where $\mathcal{D} = [\boldsymbol{\eta}^T, \mathbf{y}^T]^T$, we have $\mathcal{D}|\boldsymbol{\theta}, \lambda_\delta, \boldsymbol{\rho}^\delta \sim \text{N}(\mathbf{0}, \mathbf{C}_\mathcal{D})$, and $\pi(\boldsymbol{\theta}, \lambda_\delta, \boldsymbol{\rho}^\delta|\mathcal{D}) \propto \pi(\mathcal{D}|\boldsymbol{\theta}, \lambda_\delta, \boldsymbol{\rho}^\delta) \times \pi(\boldsymbol{\theta}) \times \pi(\lambda_\delta) \times \pi(\boldsymbol{\rho}^\delta)$. where $\mathbf{C}_\mathcal{D}$ is given by C_η, plus C_δ in the submatrix corresponding to $\mathbf{y}$. We explore this via MCMC.

Choosing target observations

- To optimize, we need targets exceeding achievable results. But for identifiability, targets should be near the model range. To satisfy these constraints, we need a rough estimate of the Pareto front.
- We achieve this by a preliminary round of calibration, with a weak prior on λ_δ. This exploits problems of identifiability in the Kennedy-O'Hagan calibration framework[1] to explore the Pareto front.
- Using the results of preliminary calibration, we select a performance target near the model range.

Estimated Pareto front with desired observation
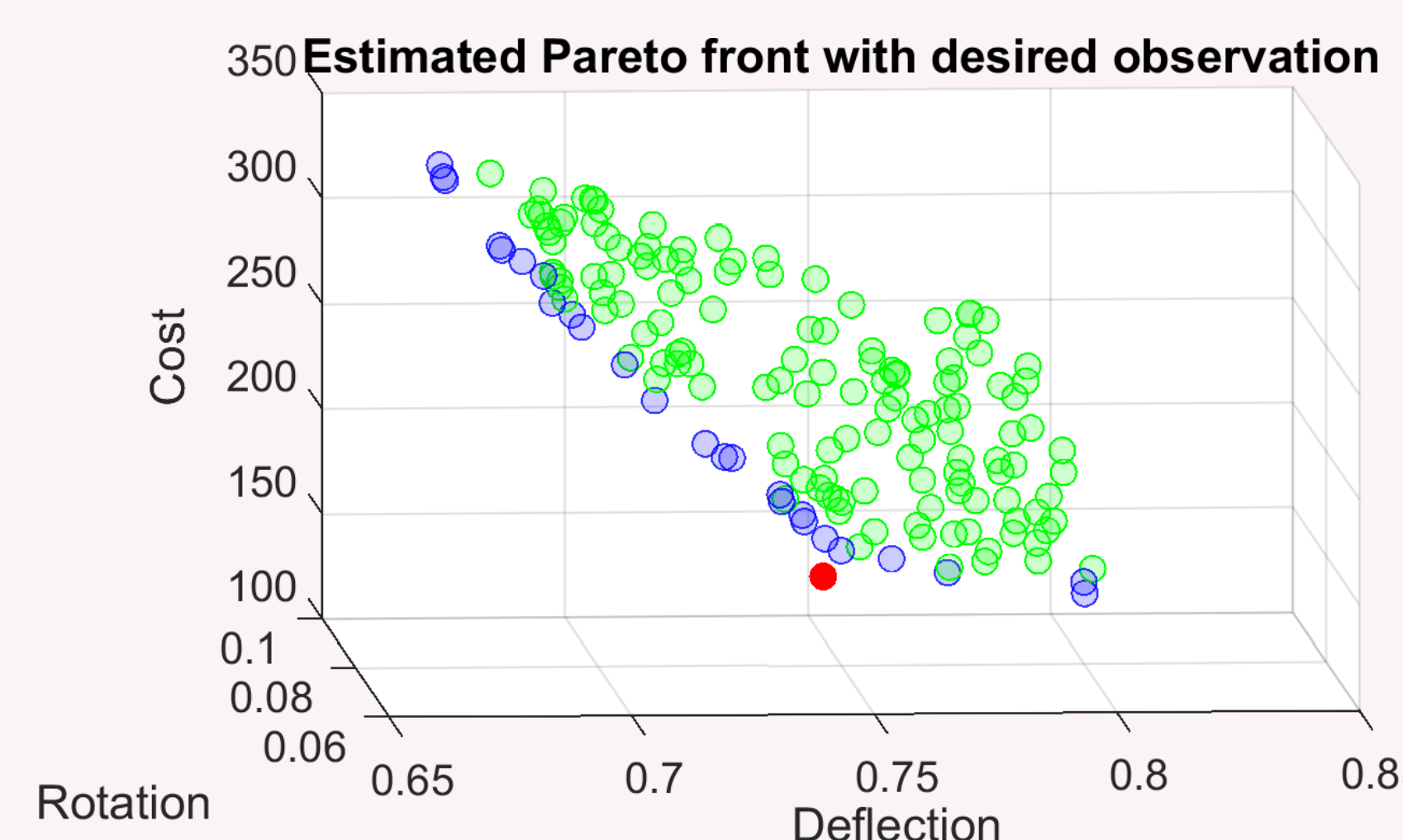
Central idea

Researchers look to computer experiments where physical experimentation is difficult or impossible[2, 3]. Previous explorations of computer model calibration have approached calibration as a matter of bringing a computer model into agreement with physical reality[4, 1, 5, 6]. **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 observations" which describe the performance one hopes to achieve in the simulated system.

Artificial system example

Model outcomes on normalized scale
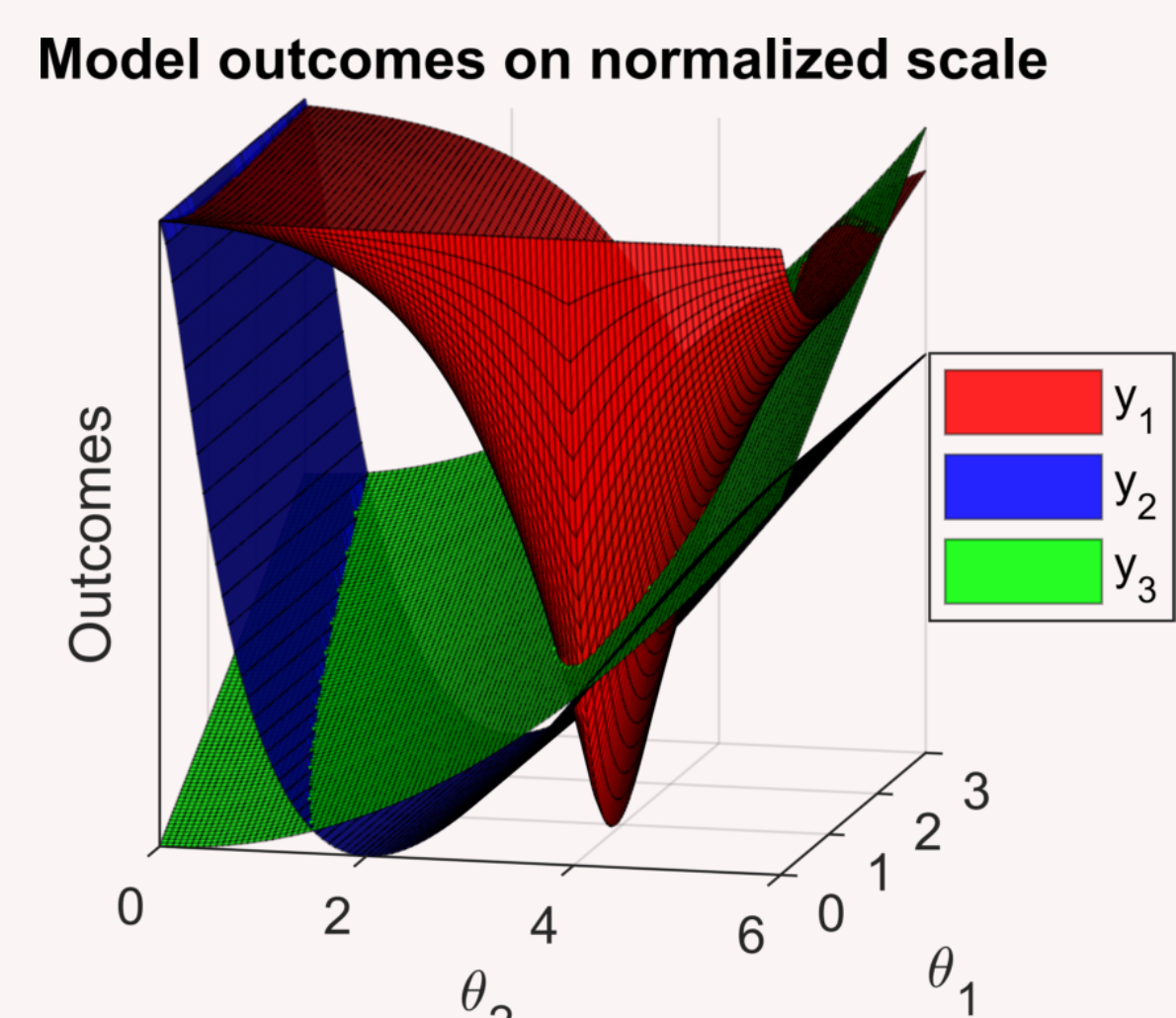
- Consider $f : [1.95, 2.05] \times [0, 3] \times [0, 6] \to \mathbb{R}^3$ where the latter two inputs are treated as calibration parameters. We seek to minimize the three model outputs:

$$f_1(x, \theta_1, \theta_2) = \left(\theta_1 \exp\left(-\left(\theta_1 + |\theta_2 - \frac{\pi x}{2}|\right)\right) + 1\right)^{-1}$$

$$f_2(x, \theta_1, \theta_2) = \left(\theta_2^{x-1} \exp\left(-0.75\theta_2\right) + 1\right)^{-1}$$

$$f_3(x, \theta_1, \theta_2) = 15 + 2\theta_1 + \frac{\theta_2^2}{4}$$

- Initially, the performance target of $[0, 0, 0]$ was chosen. To improve the identifiability of the optimal region, we used a preliminary round of calibration to update this to a target of $[0.71, 0.71, 17.92]$, constant w.r.t. x.

Artificial example results

Posterior θ samples
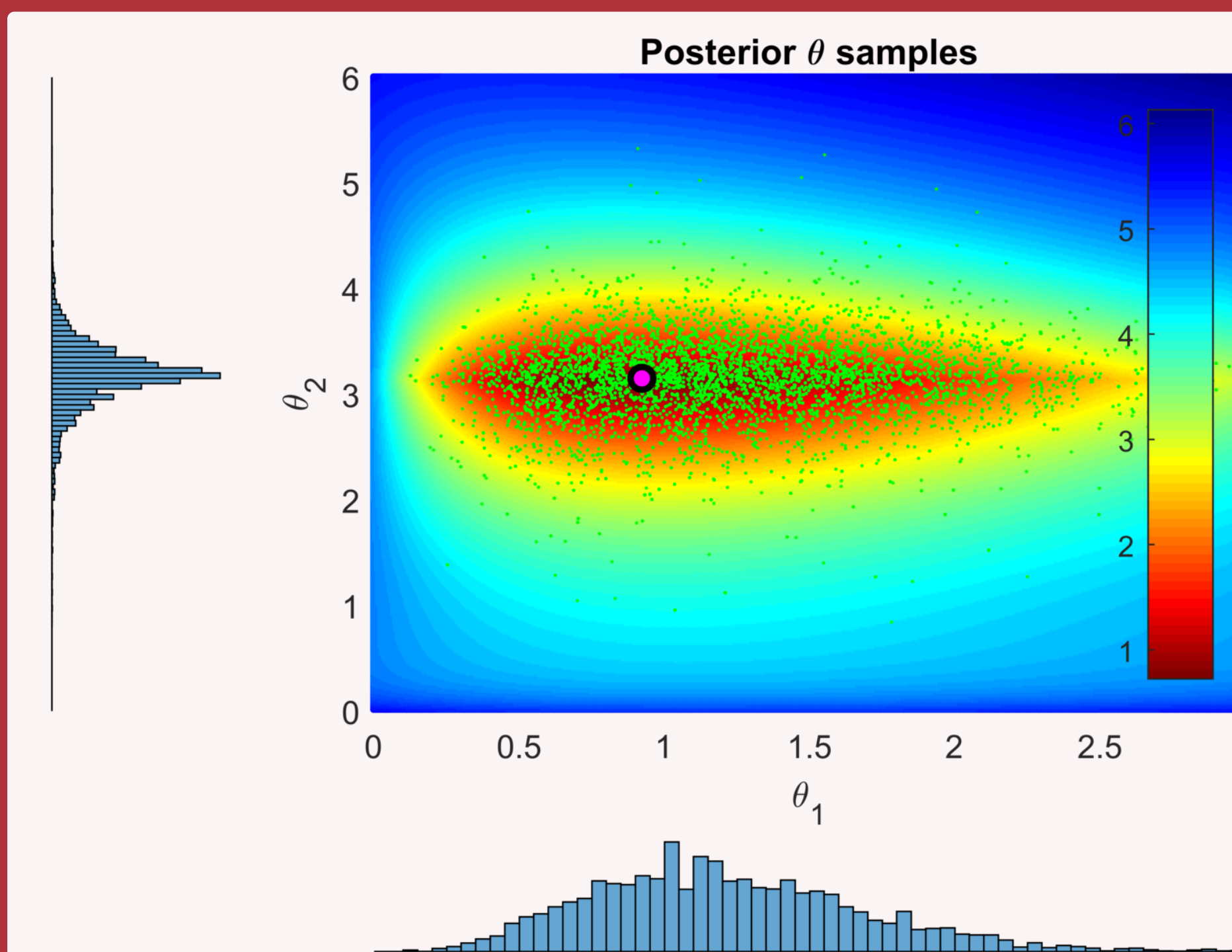
- The heatmap gives the Euclidean distance (on the standardized scale), at each point of the support of $\boldsymbol{\theta}$, of the model output at that point from the desired output $[0.71, 0.71, 17.92]$.
- The true optimum is shown as a purple dot. The green points are samples drawn via MCMC from the posterior distribution of $\boldsymbol{\theta}$, with marginal histograms also shown.

Wind turbine blade application

We calibrate to find parameters for optimal performance and cost of a wind turbine blade of fixed geometry. We rely on a finite element simulator of the blade cost and performance.
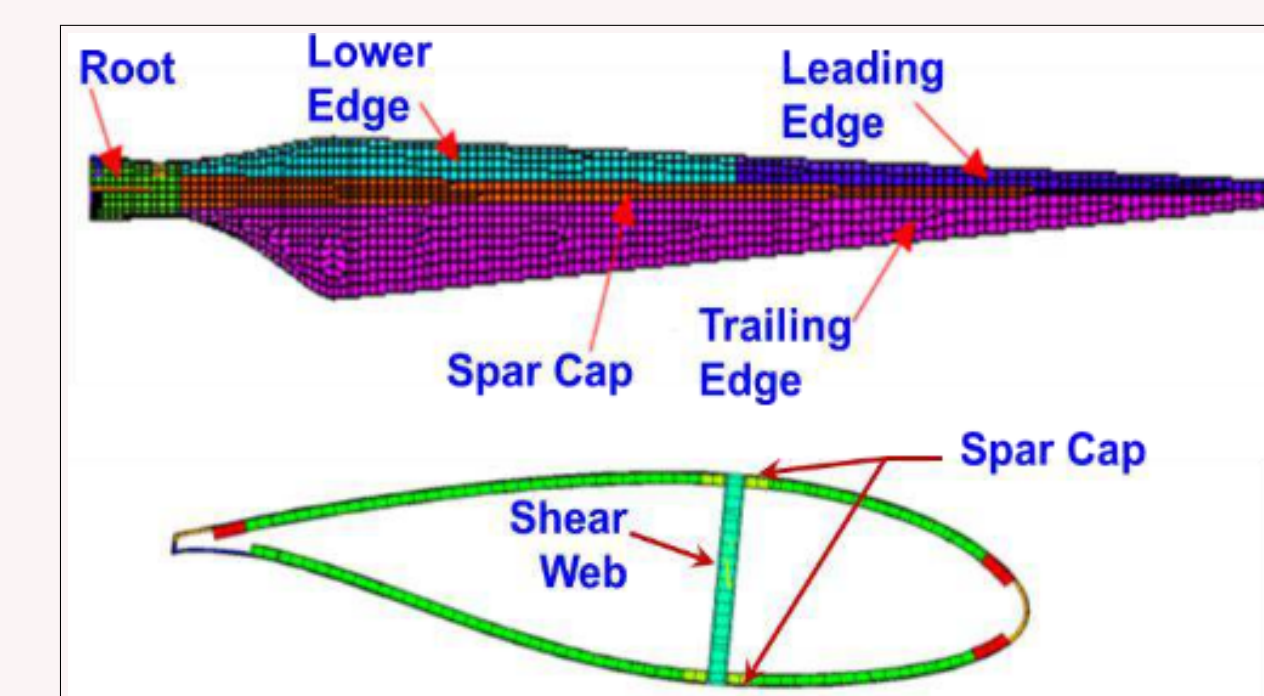
- Calibration inputs: volume fraction, thickness of blade material (in mm). Control input: temperature (in Kelvin). Support of the calibration inputs is known to be $[0.2, 0.6] \times [10, 25]$.
- Outputs are tip deflection, rotation, and cost; the design goal is to minimize these.
- Model utilizes `ANSYS` simulation software; computation cost is too high for use in MCMC.

Wind turbine blade results

- The below figure gives the posterior distribution of the calibration inputs. The (uniform) prior distributions are given by the red dashed line.

Volume fraction / Thickness (mm)
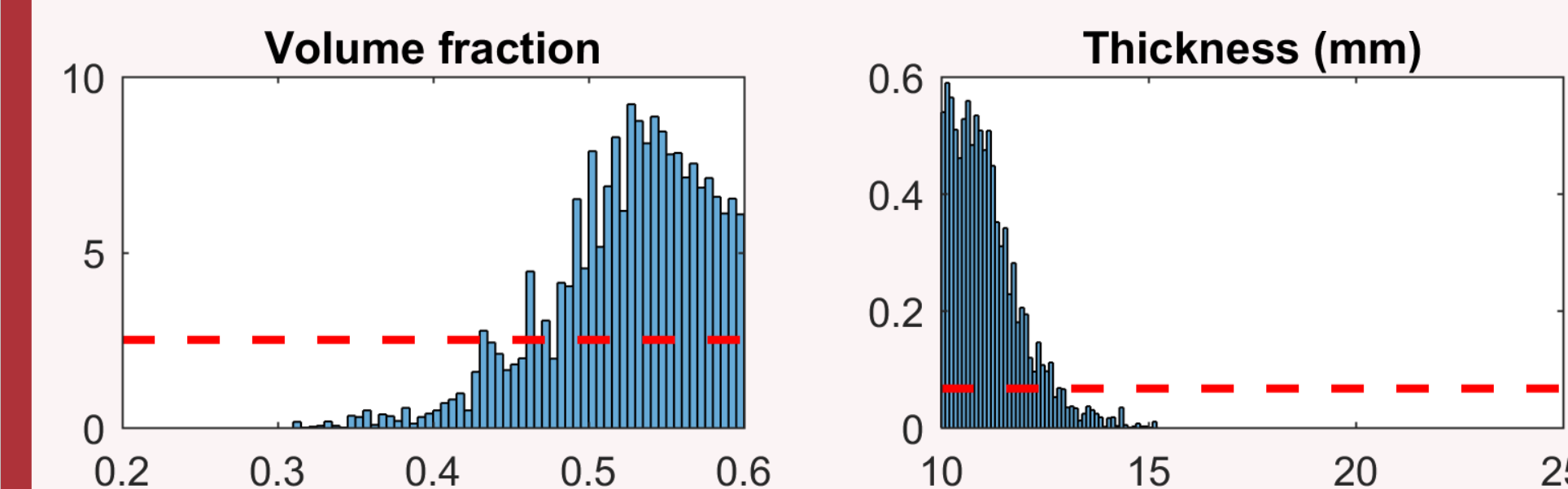
- The below figure gives the prior and posterior predictive distributions for the model. The dashed black lines show the desired observation.
- Note that it is to be expected that, as seen here, the posterior predictive distribution does not peak at the desired observation, since the desired observation was intentionally selected to lie outside of the model range.


Prior (red) and posterior (blue) predictive distributions
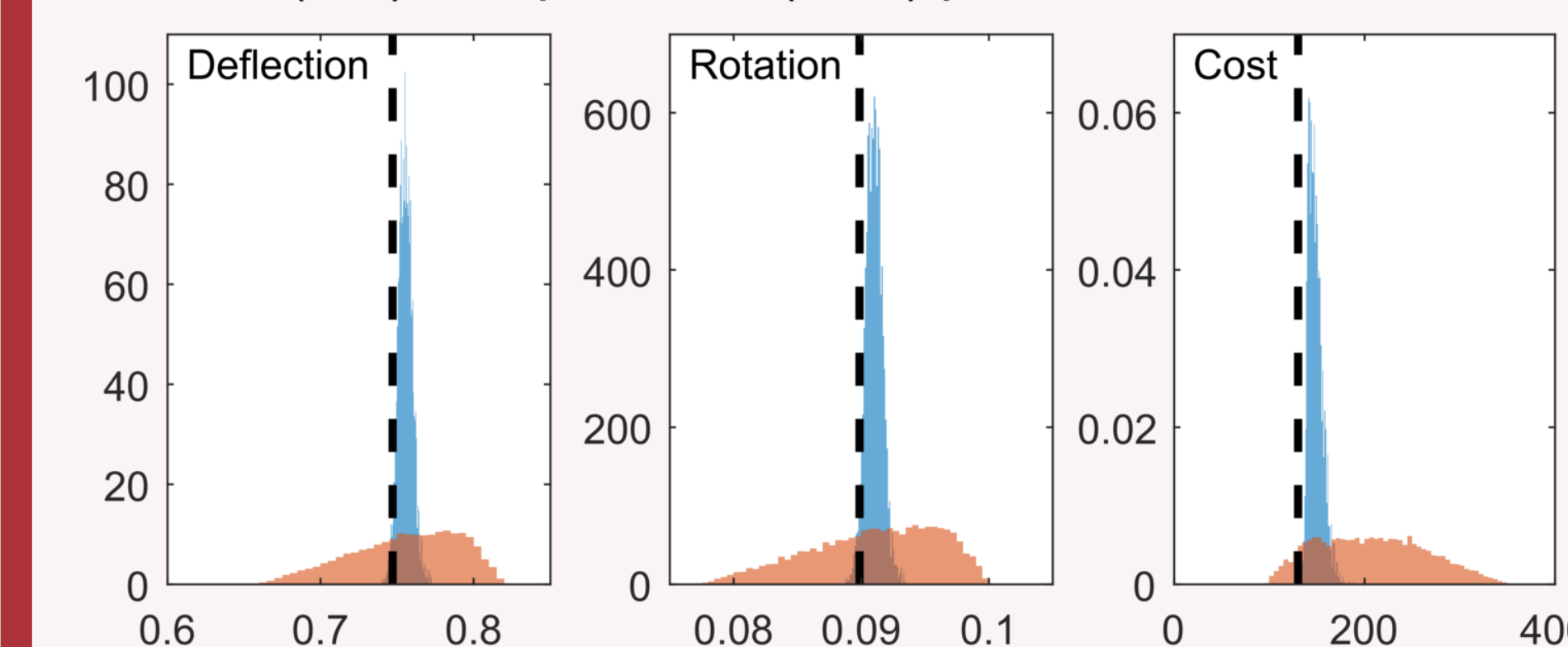
Pareto bands

- Rather than calibrating to a single set of desired observations, calibration can be performed at each point of a grid over $q - 1$ of the q model outputs.
- This permits one to use the calibration procedure to get a comprehensive picture of the Pareto front of the model, complete with uncertainty bands.
- This approach is illustrated here in the wind turbine application. For simplicity, rotation was removed from the model, so that only deflection and cost are considered. We drew a one-dimensional grid over the range of cost outputs from the model, and performed calibration at each point in the grid.
- At each point, we treat cost as known up to measurement error, and attempt to minimize deflection.
- The below right plot shows the resulting estimate of the Pareto front for the model, complete with uncertainty bands.

Posterior estimate vs. target cost, with 90% credible interval
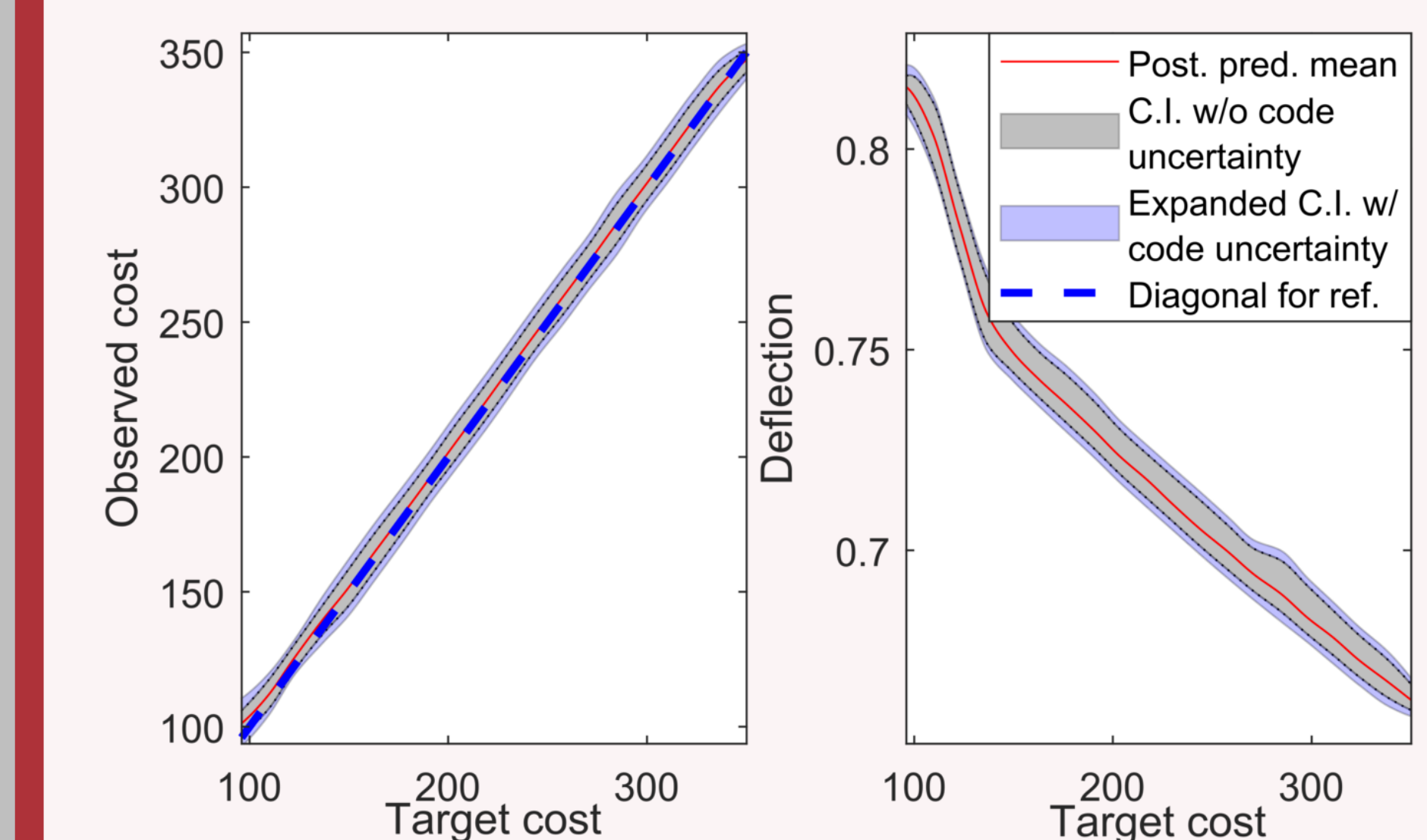
- The left plot is included to verify that the "known" cost was achieved in each calibration; i.e., that the target cost in the right plot faithfully represents the true cost.

References

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