Nonparametric Functional Calibration of Computer Models

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Computer Experiments

- Many phenomena studied in engineering and science are driven by complex processes.
- Physical experiments may be difficult to conduct because of economic, technical, or ethical limitations.
- Today, the use of computer simulations as proxies for resource-intensive physical data is common.
- Examples:
  - Large-scale climate models
  - Plastic deformation of materials under extreme conditions
  - Performance of experimental prosthetic devices

Sacks et al. (1989), Santner et al. (2003)

Computer Model Calibration

- Utility of any computer model depends on the model's fidelity to reality
- Model Calibration: Determine appropriate values of parameters in the computer code so that the output closely approximates physical observations
- Experimental design (control) settings: $\boldsymbol{x}_i \in [0,1]^{d_x},\ i = 1, \ldots, N,\ d_x \geq 1$
- True parameter values under which the computer model agrees with reality: $\boldsymbol{\theta}$
- Representation:

$$\underbrace{y(\boldsymbol{x}_i)}_{\text{field data}} = \underbrace{\eta(\boldsymbol{x}_i, \boldsymbol{\theta})}_{\text{computer output}} + \underbrace{\epsilon_i}_{\text{Gaussian error}}$$

- The Bayesian approach is to assign $\boldsymbol{\theta}$ a prior and base predictions on the posterior predictive distribution of y_i
- Priors elicited from subject matter experts are often necessary to account for weakly identifiable parameters

Kennedy and O'Hagan (2001), Bayarri et al. (2007), Higdon et al. (2008)

Functional Calibration

- Standard practice is to assume $\boldsymbol{\theta}$ is fixed throughout the domain of control inputs
- Often in practice, the best settings for the calibration parameters may change with different control inputs
- Goal: Model calibration parameters as smooth nonparametric functions of the control inputs, while accounting for expert-elicited prior constraints

Fugate et al. (2006), Atamturktur et al. (2015), Pourhabib et al. (2015), Plumlee et al. (2016)

Contribution: State-Aware Calibration

- Partition parameters into functional ($\boldsymbol{\theta}_1(\boldsymbol{x})$) and constant ($\boldsymbol{\theta}_2$) parameters and assume independence *a priori*:

$$\pi(\boldsymbol{\theta}(\boldsymbol{x})) = \pi_1(\boldsymbol{\theta}_1(\boldsymbol{x}))\pi_2(\boldsymbol{\theta}_2)$$

- Nonparametric Gaussian process model for $\boldsymbol{\theta}(\cdot)$
- Scale $\boldsymbol{\theta}$ to lie in the unit hypercube to honor expert-elicited bounds
  - Use an appropriate link function to avoid boundary issues

$$g(\theta_{1i}(\cdot)) \overset{\text{indep.}}{\sim} \mathcal{GP}(\mu_{\theta,i},\ \lambda_{\theta,i}^{-1} R_i(\cdot,\cdot))$$

$$R_i(\mathbf{x}, \mathbf{x}') = \exp\left\{-4\sum_{k=1}^{d_x} \gamma_{\theta,i,k}|x_k - x_k'|^2\right\}$$

where $g : (0,1) \to \mathbb{R}$ is one-to-one and differentiable, $\lambda_{\theta,i}$ are the unknown precisions, and $\gamma_{\theta,i,k}$ controls the smoothness of $\theta_{1i}(\cdot)$ along the k^{th} direction

McCullagh and Nelder (1989), Rasumssen and Williams (2006)

Ex: Two-Parameter Model with Scalar Control

Proposed model:

$$\begin{aligned}
\mathbf{y} \mid \boldsymbol{\theta}^{(\mathbf{x})},\ \lambda_y &\sim N_N(\boldsymbol{\eta}(\boldsymbol{\theta}^{(\mathbf{x})}),\ \lambda_y^{-1}\mathbf{I}) \\
\lambda_y &\sim \text{Ga}(a_y,\ b_y),\quad a_y, b_y > 0 \\
g(\theta_1(\cdot)) \mid \lambda_\theta,\ \rho_\theta &\sim \mathcal{GP}(\mu_\theta,\ \lambda_\theta^{-1}R_{\rho_\theta}(\cdot,\cdot)),\quad -\infty < \mu_\theta < \infty \\
\theta_2 &\sim \text{Unif}(0, 1) \\
\lambda_\theta &\sim \text{Ga}(a_\theta,\ b_\theta),\quad a_\theta, b_\theta > 0 \\
\rho_\theta &\sim \text{Beta}(1,\ b_\theta),\quad b_\theta > 0,
\end{aligned}$$

where $\boldsymbol{\eta}(\boldsymbol{\theta}^{(\mathbf{x})}) = (\eta(x_1, \theta_1(x_1), \theta_2), \ldots, \eta(x_N, \theta_1(x_N), \theta_2))^T$, $\boldsymbol{\theta}_1^{(\mathbf{x})} = (\theta_1(x_1), \ldots, \theta_1(x_N))^T$, and $R_{\rho_\theta}(x,\ x') = \rho_\theta^{4(x-x')^2}$

- Enforce smoothness through choice of b_θ
  - E.g., $b_\theta = 0.1$ or $b_\theta = 0.2$
- Standardized data $\Rightarrow$ concentrate λ_y near one

Atamturktur and **B** (2015), **B** and Atamturktur (2016)

Implementation (MCMC)

- Eliminate boundary constraints with $\xi = \log(-\log(\theta_2))$ and $\nu = \log(-\log(\rho_\theta))$
- Metropolis proposal $(g(\theta_1^\dagger(x_1)), \ldots, g(\theta_1^\dagger(x_N)))^T \sim MVN$ with correlation matrix dependent upon the current value of ρ_θ
- Observed design points close together $\Rightarrow$ correlation matrix is numerically unstable
  - Add a 'nugget': $\mathbf{R}_{\nu,\delta} := \mathbf{R}_\nu + \delta\mathbf{I}$

Tierney (1994), Neal (1998, 2011), Qian and Wu (2008), Ranjan et al. (2011)

Simulation Study

- Truth: $y(x_i) = \underbrace{c_1(x_i)}_{=2\sqrt{x_i}} + \underbrace{c_2}_{=2.5} x_i^2 + \varepsilon_i,\quad \varepsilon_i \overset{\text{iid}}{\sim} N(0,\ 0.05^2)$
- Computer model: $\eta(x, t_1, t_2) = t_1 + t_2 x^2$
- Field data generated at $\mathbf{x} = (0.00, 0.05, 0.10, \ldots, 0.90, 0.95)^T$; responses $\mathbf{y}^* = (y(0.45), \ldots, y(0.65))^T$ held out for validation

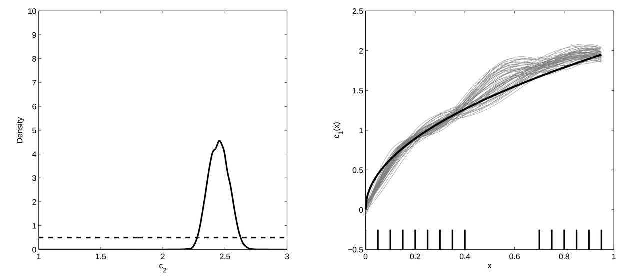

Figure : Posteriors of $c_1(\cdot)$ and c_2 under the logit link with constraints on the boundary values of $c_1(\cdot)$. The dashed and solid curves in the left panel are the prior and posterior densities of c_2, respectively. The thick line in the right panel is the true function $c_1(\cdot)$.

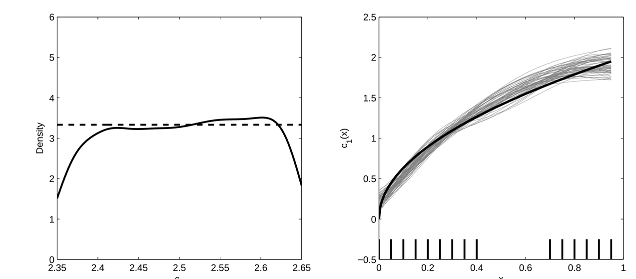

Figure : Posteriors of $c_1(\cdot)$ and c_2 with logit link and tight prior bounds on c_2. The dashed and solid curves in the left panel are the prior and posterior densities of c_2, respectively.

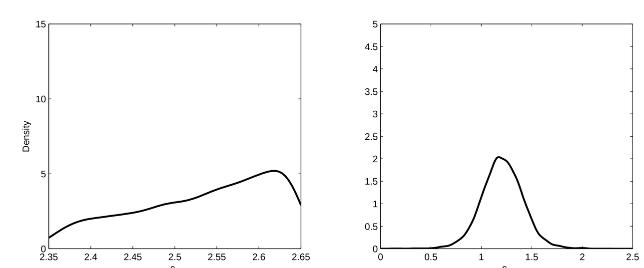

Figure : Smoothed approximate posterior distributions of c_2 and c_1 when replacing the GP prior on $\theta_1(\cdot)$ with $\theta_1 \sim$ Uniform.

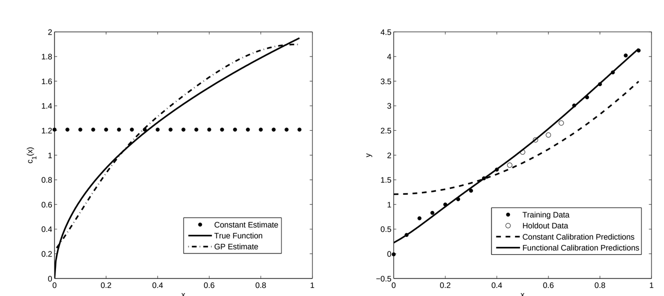

Figure : Strong disagreement between calibrated code and field data when assuming constant parameters

Summary

- Proposed model adequately captures functional behavior
- Erroneously assuming constant parameters can be misleading
- Similar results from logit, probit, and identity link functions

Application: VPSC Plastic Deformation

- Model for plastic deformation of viscoplastic self-consistent (VPSC) materials
- Experiments with 5182 aluminum (to which VPSC is applicable) applied strain to each specimen up to 0.6, after which the stress is recorded.
- VPSC computer code:

$$\underbrace{y}_{\text{stress}} = \eta(\underbrace{x}_{\text{temperature}},\ \underbrace{\theta_1(x)}_{\text{critical resolved shear stress}},\ \underbrace{\theta_2}_{\text{inverse rate sensitivity}}) + \epsilon$$

Lebensohn and Tomé (1993), Stout et al. (1998), Atamturktur et al. (2015)

Results

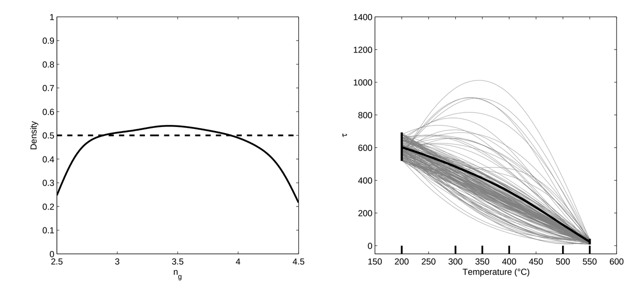

Figure : Smoothed prior and posterior histogram for inverse rate sensitivity (left panel) and sample paths drawn from the posterior of shear stress (right panel). The dark curve in the center is the pointwise mean of the sample paths; the vertical lines on the boundaries indicate the prior constraints imposed on the curves.

- Results agree with previous empirical work
- Model adequacy checks indicate modeling assumptions are consistent with experimental data

Conclusions

- Proposed approach incorporates prior information and fully accounts for uncertainty.
- Assuming constant parameters may be misleading. A researcher may include an empirical discrepancy term when functional calibration is needed.
- When to invoke state-aware calibration?
  1. Begin with conventional (all constant) calibration
  2. Systematic model bias $\Rightarrow$ consider functional relationships
  3. Sensitivity analysis to identify likely functional parameters
  4. Compare nonparametric and parametric models

Reference

Brown, D. A. and Atamturktur, S. (2018), "Nonparametric functional calibration of computer models," *Statistica Sinica*, to appear. `doi:10.5705/ss.202015.0344`

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