Quantifying Uncertainty with GPM/SA
Recent Application-Focused Extensions
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Framework for Statistical Calibration & UQ

**Gaussian Process (GP) Formulation**

- $x$ model or system inputs
- $\theta$ model calibration parameters
- $\zeta(x)$ true physical system response given inputs $x$
- $\gamma(x; \theta)$ simulator response at $x$ and $\theta$
- $\delta(x)$ discrepancy between $\zeta(x)$ and $\gamma(x; \theta)$
- $c(x)$ observation error of the experimental data

**This Framework Implemented in GPM/SA code**

Reference Implementation in Matlab, also C++ (Dakota/QUESO)
Utilities for cross-validation, sensitivity analysis, prediction with uncertainty

MCMC Sampling calibrates GPM/SA model and parameters:

$\Sigma_n = \exp\left(-\frac{1}{2} s_i (X_i - x)^T \Sigma^{-1} (X_i - x)\right)$

$\tilde{x}(\theta, \gamma(x; \theta)) \sim \exp\left(-\frac{1}{2} (y - f)^T \Sigma^{-1} (y - f)\right)$

**Important elements include:**

- Design of computer experiments
- Response emulation, including uncertainty
- Model Discrepancy
- Dimension Reduction, with Linear Basis decomposition
- Calibration of parameters to observation data

**Kronecker Designs**

Challenge:
Gaussian Process models have a basic computational limitation on number of samples $n$; the size $n$ covariance inverse is needed. One approach to mitigation is Kronecker-separable designs.

Approach is to partition the parameters $P$ into $P = [P_1, P_2]$, and create the sample design so that $X = \text{kron}(X_1, X_2)$
This means that for every sample in $X_1$, there is the full design in $X_2$. The advantage is that the inverse covariance $C^{-1}(X) = \text{kron}(C^{-1}(X_1), C^{-1}(X_2))$ can be computed efficiently.

Cosmology Application
3700 model runs treated
37 run design 100 run design

**Categorical Variables**

Challenge:
Model assumes continuous parameters with Euclidean norm. We still want to treat categorical parameters, not as independent models.

Define a parameterized covariance for categorical variables
Model can calibrate how similar response should be across categories

*Example in physics of CO$_2$ capture “Bubbling Fluidized Bed” model:*

- Four x settings (cols)
- Two output types (rows)
- Across angle (-90, 90)
- Observations in black
- 6 Parameters, Color represents categorical parameter

**Hierarchical Linked Calibration**

Challenges:
Different observation types may have different implications to parameter values and uncertainty
Different models may have different implications for an observation
It’s not realistic to expect discrepancy to be known

Upside:
- More observation groups/modes give more information about model structural error and uncertainty.

Inference model acknowledging bias terms for different observations:

$y_i = \eta(x, \theta_i) + \delta_i(x, \theta + b_i) + \epsilon_i$

The distribution of the $b_i$ can be estimated by a hierarchical modeling approach:

$y_i = \eta(x, \theta_i) + \epsilon_i$

$\theta_i \sim N(\mu_0, \sigma^2_0)$

$\mu_0 \sim U(0, 1)$

$\lambda_y = \frac{\sigma^2_y}{\sigma^2_0} \sim \Gamma(a - 1, b \to \infty)$

Across the observations/models:
- One extreme: parameters are identical
- Other extreme: parameters are independent

Generally, this reveals a source of additional uncertainty.

Examples with small parameter sets:
Calibrating a Nuclear DFT Model (see NUCLEI poster)
Calibrating Intermediate Complexity climate model:

**Posterior distribution of parameters sensitivity, ocean heat diffusion rate, aerosol forcing, comparing to observation datasets**

(Foell et al.)

GPM/SA standard model calibration, including estimating model discrepancy
GPM/SA hierarchical model calibration, with Normal hierarchical distributions on parameters.

Calibrating a parameterization shows ability to make tradeoffs

Inference from red, green, blue measures (in isolation) are strong and consistent, combine as black

Conflicting inferences from cyan, magenta measures are weak, but not entirely ruled out.