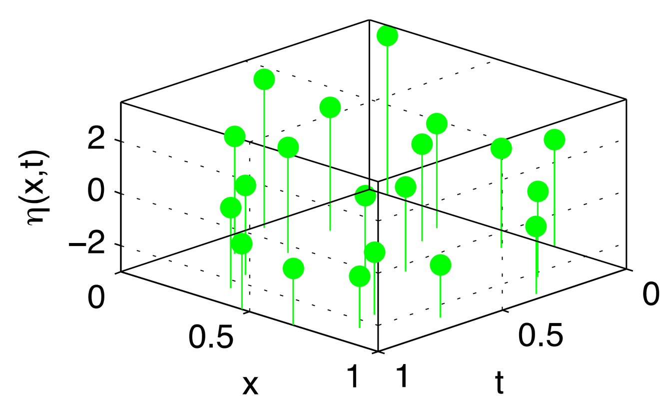
Quantifying Uncertainty with GPM/SA

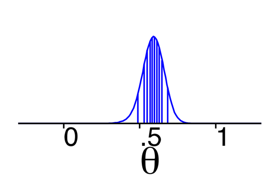
Recent Application-Focused Extensions

Dave Higdon, James Gattiker   *LANL Statistical Sciences*

Los Alamos NATIONAL LABORATORY

Framework for Statistical Calibration & UQ





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

Gaussian Process (GP) Formulation

x	model or system inputs
θ	model calibration parameters
$\zeta(x)$	true physical system response given inputs x
$\eta(x,\theta)$	simulator response at x and θ.
$y(x)$	experimental observation of the physical system
$\delta(x)$	discrepancy between $\zeta(x)$ and $\eta(x,\theta)$ may be decomposed into numerical error and bias
$e(x)$	observation error of the experimental data

$$y(x) = \zeta(x) + e(x)$$
$$y(x) = \eta(x,\theta) + \delta(x) + e(x)$$

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:

$$\Sigma_{12} = \exp\{-\beta|x_1 - x_2|^p\}$$

(GP is defined by covariance between data sites)

$$\pi(\theta, \eta(\cdot,\cdot) \,|\, y(x)) \propto L(y(x) \,|\, \eta(x,\theta)) \times \pi(\theta) \times \pi(\eta(\cdot,\cdot))$$

$$L \approx \frac{1}{\sqrt{\det(\Sigma)}} \exp\{-\frac{1}{2}(Y-f)'\Sigma^{-1}(Y-f)\}$$

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.

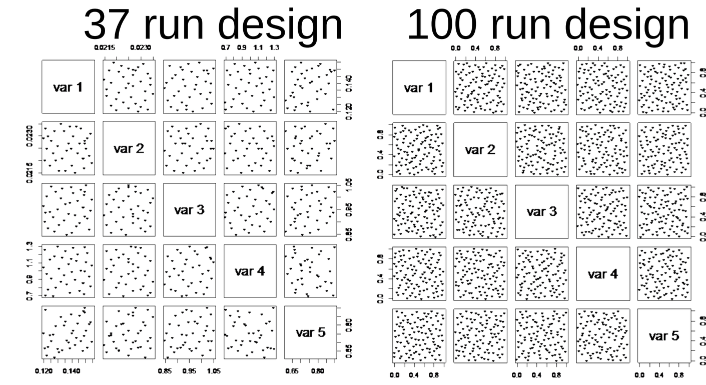
Approach is to partition the parameters P into P=[P_1 P_2], and create the sample design so that X=kron(X_1,X_2)

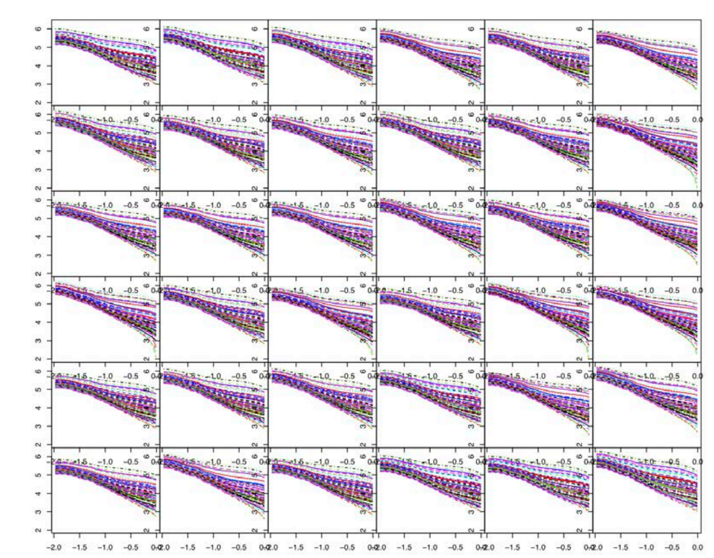
This means that for every sample in X_1, there is the full design in X_2

The advantage is that the inverse covariance $C^{-1}(X)$=kron($C^{-1}(X_1)$,$C^{-1}(X_2)$) can be computed efficiently

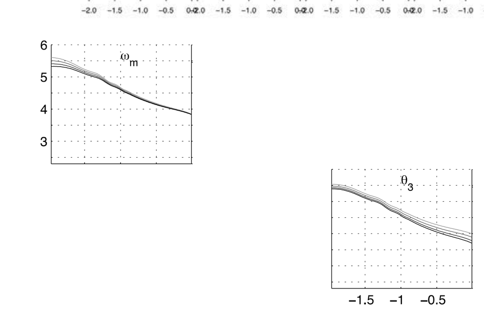
Cosmology Application

3700 model runs treated





Full-Bayes calibration computationally viable:



Categorical Variables

Challenge:

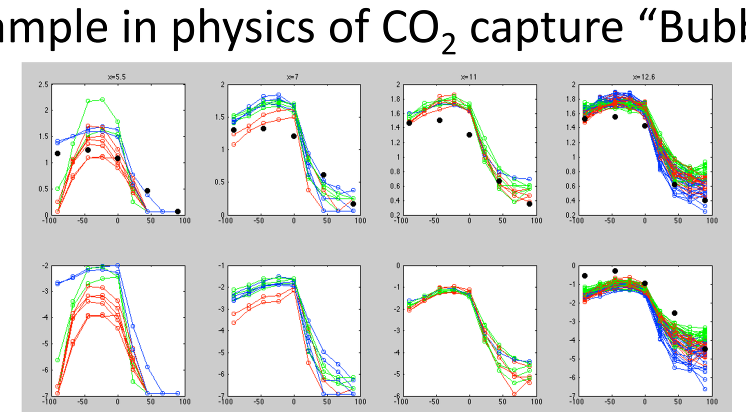
Model assumes continuous parameters with Euclidean norm.

We still want to treat categorical parameters, not as independent models.

Define a parameterized covariance for categorical variables

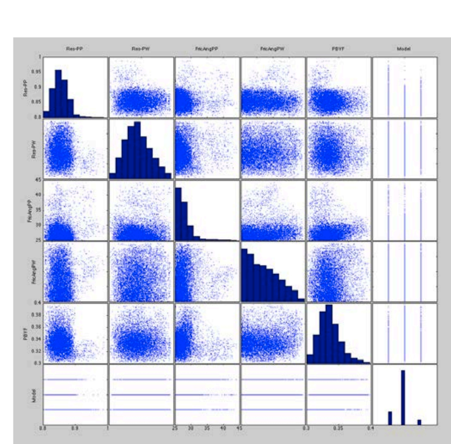
Model can calibrate how similar response should be across categories

Example in physics of CO_2 capture "Bubbling Fluidized Bed" model:



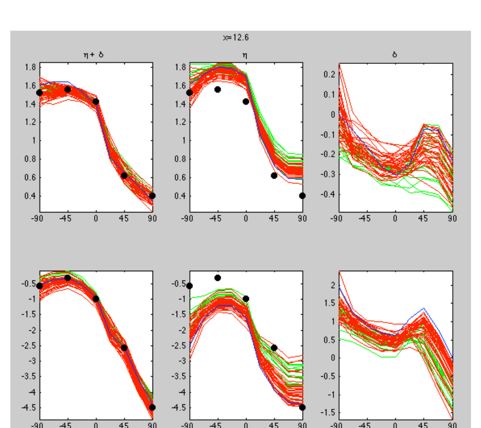
Four x settings (cols)
Two output types (rows)
Across angle (-90,90)
Observations in black

6 Parameters,
Color represents categorical parameter



Calibration prefers Cat. Level 2

Posterior prediction:



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:

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

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

$$y_i = \eta(x, \theta_i) + \epsilon_i \qquad \theta_i \propto N(\mu_\theta, \sigma_\theta^2)$$
$$\mu_\theta \propto U(0,1)$$
$$\lambda_\theta \equiv \frac{1}{\sigma_\theta^2} \propto \Gamma(a=1, b\to\infty)$$

Across the observations/models:

One extreme: parameters are identical

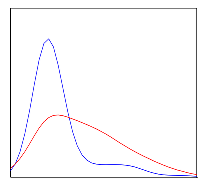
Other extreme: parameters are independent

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 distrubiton of parameters sensitivity, ocean heat diffusion rate, aerosol forcing, comparing to observation datasets
(Forest 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.