Embedded Model Error Representation

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LLNL SciDAC4 Prop Meeting
January 30, 2017

Further acknowledgements:
R. Ghanem(USC), J. Bender(LLNL), Y. Marzouk(MIT), C. Feng(MIT),
M. Eldred (SNL), C. Safta (SNL), B. Debusschere (SNL).
Model error = deviation from ‘truth’, or from a higher-fidelity model

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization

- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions

- Inverse modeling context
  - Given experimental or higher-fidelity model data, estimate the model error
Motivation

Given noisy data – Gaussian noise

\[ y = g_{\text{true}}(x) + \epsilon \]
Employ Bayesian inference to fit an exponential model – $y_m = f(x, \lambda)$

Discrepancy between data and prediction presumed exclusively due to \textit{i.i.d.} Gaussian data noise – $y = f(x, \lambda) + \epsilon_d$

Plotted:
- Posterior density on the parameters
- Predictive mean and standard deviation
Employ Bayesian inference to fit an exponential model – \( y_m = f(x, \lambda) \)

Discrepancy between data and prediction presumed exclusively due to \( i.i.d. \) Gaussian data noise – \( y = f(x, \lambda) + \epsilon_d \)

True model \( g(x) \) – dashed-red – differs from fit model \( f(x, \lambda) \)

Actual discrepancy includes both data and model errors
Motivation

- Increasing number of data points decreases posterior and predictive uncertainty
- We are increasingly sure about predictions based on the *wrong* model
Motivation

- Increasing number of data points decreases posterior and predictive uncertainty
- We are increasingly sure about predictions based on the *wrong* model
Motivation

- If the model has structural uncertainty, more data leads to biased and overconfident results
- We want to quantify model-vs-truth discrepancy in a rigorous and systematic way
  - Cannot ignore model error
Explicit model discrepancy: issues for physical models

\[ y_i = f(x_i; \lambda) + \delta(x_i) + \epsilon_i \]

- Explicit additive statistical model for model error \( \delta(x) \) [Kennedy-O’Hagan, 2001]
- Potential violation of physical constraints
- Disambiguation of model error \( \delta(x_i) \) and data error \( \epsilon_i \)
- Calibration of model error on measured observable does not impact the quality of model predictions on other QoIs
- Physical scientists are unlikely to augment their model with a statistical model error term on select outputs
  - Calibrated predictive model: \( f(x; \lambda) + \delta(x) \) or \( f(x; \lambda) \)?
- Problem is highlighted in model-to-model calibration \( (\epsilon_i = 0) \)
  - no a priori knowledge of the statistical structure of \( \delta(x) \)
Model error embedding: key idea

Ideally, modelers want predictive errorbars: inserting randomness on the outputs has issues, so...

- Cast input parameters $\lambda$ as a random variable $\Lambda$

  \[
  y_i = f(x_i; \Lambda) + \epsilon_i
  \]

- Generalize parameter forms,

  \[
  y_i = f(x_i; \Lambda(x_i)) + \epsilon_i
  \]

- More generally, explore additional parameterizations,

  \[
  y_i = \tilde{f}(x_i; \lambda, \Theta) + \epsilon_i
  \]
Model error embedding: key idea

Ideally, modelers want predictive errorbars: inserting randomness on the outputs has issues, so...

- Cast input parameters $\lambda$ as a random variable $\Lambda$

$$y_i = f(x_i; \Lambda) + \epsilon_i$$

Black-box

... even simpler, *additive correction term*

$$y_i = f(x_i; \lambda + \delta(\alpha, \xi)) + \epsilon_i$$

- Infer the parameters of the correction ($\alpha$) with the model parameters ($\lambda$)

- Stochastic dimension $\xi$ corresponds to model error
Model error embedding: key idea

Augment input parameters $\lambda$ with additive term $\delta(\alpha, \xi)$

$$y_i = f(x_i; \lambda) + \delta(x_i) + \epsilon_i \quad \rightarrow \quad y_i = f(x_i; \lambda + \delta(\alpha, \xi)) + \epsilon_i$$

- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property

- Allows placement of model error term in locations where key modeling assumptions and approximations are made
  - as a correction or high-order term
  - as a possible alternate phenomenology

- Naturally preserves model structure and physical constraints
Model error embedding – Bayesian density estimation

\[ y_i = f(x_i; \lambda + \delta) + \epsilon_i \]

- Parametrize embedded random variable \( \delta \):
  - PDF form \( \pi_\delta(\cdot; \alpha) \)
  - Polynomial Chaos (PC): \( \delta = \sum_k \alpha_k \Psi_k(\xi) \)
    - \( \delta_1 = \alpha_{11} \xi_1 \)
    - \( \delta_2 = \alpha_{21} \xi_1 + \alpha_{22} \xi_2 \)
    - \[ \vdots \]
    - \( \delta_d = \alpha_{d1} \xi_1 + \alpha_{d2} \xi_2 + \cdots + \alpha_{dd} \xi_d \)
  - Multivariate Normal (MVN): \[
    \begin{cases}
    \delta_1 = \alpha_{11} \xi_1 \\
    \delta_2 = \alpha_{21} \xi_1 + \alpha_{22} \xi_2 \\
    \vdots \\
    \delta_d = \alpha_{d1} \xi_1 + \alpha_{d2} \xi_2 + \cdots + \alpha_{dd} \xi_d
    \end{cases}
  \]

- Inverse modeling context
  - Parameter estimation of \( \lambda \) \( \Rightarrow \) parameter estimation of \( \tilde{\alpha} = (\lambda, \alpha) \)

- Bayesian formulation

\[
p(\tilde{\alpha}|y) \propto L_y(\tilde{\alpha}) p(\tilde{\alpha})
\]

- Posterior
- Likelihood
- Prior

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Model error embedding – likelihood options

Prior \( p(\lambda, \alpha) \)

\[ \lambda + \delta(\alpha; \xi) \]

Prob. model for \( \delta \)

\[ f(x_i; \lambda + \delta) \]

Embedded model

Likelihood \( p(y|\alpha) \)

\[ y_i = g(x_i) + \epsilon_i \]

Data

Posterior \( p(\lambda, \alpha|y) \)

- Infer \( \hat{\alpha} = (\lambda, \alpha, \sigma_D) \)

- Data generation model; to aid likelihood \( p(y|\hat{\alpha}) \) construction

\[
y_i = f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i = f \left( x_i, \lambda + \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d) \right) + \sigma_D \xi_{d+i} = \]

\[
[NISP] \approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_D \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha})
\]

- Full PC germ \( \hat{\xi} = (\xi_1, \ldots, \xi_d, \xi_{d+1}, \ldots, \xi_{d+N}) \)

Model error Data noise

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Model error embedding – likelihood options

- Data generation model; to aid likelihood $p(y|\hat{\alpha})$ construction

$$y_i = f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i =$$

$$= f \left( x_i, \lambda + \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d) \right) + \sigma_D \xi_{d+i} =$$

[NISP] $$\approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_D \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha})$$

- Full Likelihood: $L(\hat{\alpha}) = p(y|\hat{\alpha}) = p(y_1, \ldots, y_N|\hat{\alpha}) = \pi(y)$

  - Degenerate if no data noise
  - Requires multivariate KDE or high-d integration
  - Gaussian approximation:
    $$L(\hat{\alpha}) \propto \exp \left(-\frac{1}{2}(y - \mu(\hat{\alpha}))^T \Sigma^{-1}(\hat{\alpha})(y - \mu(\hat{\alpha}))\right)$$
  - Non-intrusive spectral projection (NISP) relieves the expense and provides easy access to mean $\mu(\alpha)$ and covariance $\Sigma(\hat{\alpha})$
Model error embedding – likelihood options

- Data generation model; to aid likelihood $p(y|\hat{\alpha})$ construction

$$y_i = f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i =$$

$$= f\left(x_i, \lambda + \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d)\right) + \sigma_D \xi_{d+i} =$$

$$[\text{NISP}] \approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_D \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha})$$

---

- Marginalized Likelihood:

$$L(\hat{\alpha}) = p(y|\hat{\alpha}) \approx \prod_{i=1}^{N} p(y_i|\hat{\alpha}) = \prod_{i=1}^{N} \pi(y_i)$$

  - Requires univariate KDE
  - Neglects built-in correlations
  - Gaussian approximation:

$$L(\hat{\alpha}) \propto \exp\left(-\frac{1}{2} \sum_{i=1}^{N} \Sigma^{-1}_{ii}(\hat{\alpha})(y_i - \mu_i(\hat{\alpha}))^2\right)$$
Model error embedding – likelihood options

- Data generation model; to aid likelihood \( p(y|\hat{\alpha}) \) construction

\[
y_i = f(x_i, \lambda + \delta(\alpha, \xi)) + \epsilon_i = \\
= f \left( x_i, \lambda + \sum_k \alpha_k \Psi_k(\xi_1, \ldots, \xi_d) \right) + \sigma_D \xi_{d+i} = \\
[\text{NISP}] \approx \sum_k f_{ik}(\alpha) \Psi_k(\xi_1, \ldots, \xi_d) + \sigma_D \xi_{d+i} = h_i(\hat{\xi}; \hat{\alpha})
\]

- Approximate Bayesian Computation (ABC): \( L(\hat{\alpha}) = \frac{1}{\epsilon} K \left( \frac{\rho(S_M, S_D)}{\epsilon} \right) \)
  - Mean of \( f(x_i; \lambda + \delta) \) is “centered” on the data
  - The width of the distribution of \( f(x_i; \lambda + \delta) \) is consistent with the spread of the data around the nominal model prediction

\[
L(\hat{\alpha}) \propto \exp \left( -\frac{1}{2\epsilon^2} \sum_{i=1}^{N} \left[ (\mu_i(\hat{\alpha}) - y_i)^2 + (\sqrt{\sum_{ii}(\hat{\alpha})} - \gamma |\mu_i(\hat{\alpha}) - y_i|)^2 \right] \right)
\]
Non-intrusive spectral projection (NISP) will allow
- Posterior/pushed-forward predictions
- Easy access to first two moments:

\[ \mu(x; \alpha) = f_0(x; \alpha), \quad \sigma^2(x; \alpha) = \sum_{k>0} f_k^2(x; \alpha) ||\Psi_k||^2 \]

**Predictive mean**

\[ \mathbb{E}[y(x)] = \mathbb{E}_\alpha[\mu(x; \alpha)] \]

**Decomposition of predictive variance**

\[ \nabla[y(x)] = \mathbb{E}_\alpha[\sigma^2(x; \alpha)] + \nabla_\alpha[\mu(x; \alpha)] \]

\( \text{Model error} \quad \text{Posterior error} \)
Model Error – Predictions at data locations

\[ f(x_i; \lambda + \sum_k \alpha_k \Psi_k(\xi_1:d)) + \sigma_D \xi_{i+d} = \sum_k f_k(x_i; \alpha) \Psi_k(\xi_1:d) + \sigma_D \xi_{i+d} \]

- Non-intrusive spectral projection (NISP) will allow
  - Likelihood computation
  - Easy access to first two moments:
    \[ \mu(x_i; \alpha) = f_0(x_i; \alpha), \quad \sigma^2(x_i; \alpha) = \sum_{k>0} f_k^2(x_i; \alpha) \|\Psi_k\|^2 \]

- Predictive mean
  \[ \mathbb{E}[y(x_i)] = \mathbb{E}_\alpha[\mu(x_i; \alpha)] \]

- Decomposition of predictive variance
  \[ \nabla[y(x_i)] = \mathbb{E}_\alpha[\sigma^2(x_i; \alpha)] + \nabla_\alpha[\mu(x_i; \alpha)] + \sigma_d^2 \]

  - Model error
  - Posterior/Data error
More data leads to ‘leftover’ model error

Calibrating a quadratic \( f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2 \)

w.r.t. ‘truth’ \( g(x) = 6 + x^2 - 0.5(x + 1)^{3.5} \) measured with noise \( \sigma = 0.1 \).

Summary of features:

- Well-defined model-to-model calibration
- Model-driven discrepancy correlations
- Respects physical constraints
- Disambiguates model and data errors
- Calibrated predictions of multiple QoIs
Challenges

- Density estimation is more challenging than parameter estimation
  - Inverse problem is ill-posed or intractable
    ⇒ Employ approximate or empirical likelihoods

- Potentially a high-dimensional Bayesian problem
  - Full posterior may be inaccessible...
    ⇒ Resort to optimization algorithms in no-noise case
  - ... or hard to sample from
    ⇒ Adaptive MCMC algorithms, Likelihood-informed subspaces

- Sparse data or expensive high-fidelity simulations
  - With low information content, calibration may struggle
    ⇒ More informative priors/regularization
Summary

- Represent, quantify and propagate physical model errors
- Parameter estimation \(\Rightarrow\) density estimation
- Bayesian machinery to find parameters of the PDFs
- Approximate/empirical likelihoods impose constraints of interest
- Differentiates from data noise; allows model-to-model calibration
- Implemented in UQTk (www.sandia.gov/UQToolkit)
- Applied to chemical kinetics, transport modeling, LES computations...


- Optimal design for maximum information
- Optimal embedding
- Bayesian problem still hard; MCMC, priors, ...
- Hierarchical Bayesian viewpoint
- More intrusive embedding; problem specific
Applications
Model-to-model calibration: ignition model

- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model

Data: ignition time; range of initial $T$ & equivalence ratio

Single-step model:

$$\mathcal{R} = [\text{CH}_4][\text{O}_2]k_f$$

$$k_f = A \exp(-E/R^0T)$$

$$(\ln A, E) = \sum_k \alpha_k \Psi_k(\xi)$$
Model-to-model calibration: ignition model

Calibrated uncertain fit model is consistent with the detailed-model data.

Over the range of \((T^0, \Phi)\):
- MAP predictive mean ignition-time is centered on the data
- MAP predictive stdv is consistent with the scatter of the data

K. Sargsyan, H.N. Najm, and R. Ghanem
"On the Statistical Calibration of Physical Models"
TransCom3 Experiment of \( CO_2 \) Flux Inversion

[Gurney et al., Tellus B, 2003]

- Observations \( \mathbf{d} \) at \( N = 77 \) sites around the world
- Inverse problem: find fluxes \( \mathbf{s} \) at \( M = 22 \) locations
- Linearized ‘response’ model \( \mathbf{R} \), such that \( \mathbf{d} \approx \mathbf{R}\mathbf{s} \)

\[
\mathbf{d} = \mathbf{R}\mathbf{s} + \epsilon_d
\]

- Model \( \mathbf{R} \) is never perfect thus contaminating the inversion
- The inferred values of \( \mathbf{s} \) compensate for model deficiencies
- \( \epsilon_d \) is meant to capture data errors, but is ‘entangled’ with model errors
Consider 14 different response models $R$

Infer fluxes $s$, given measurements $d$ to satisfy $d \approx Rs$

- Conventional additive Gaussian error (least-squares): $d = Rs + \xi$
- Embed probabilistic model for fluxes $s$: $d = R(\mu_s + C_s \xi)$
Consider 14 different response models \( R \):

- MATCH.bruhwiler
- MATCH.chen
- MATCH.law
- NIES.maksyutov
- NIRE.taguchi
- RPN.yuen
- SKYHI.fan

Infer fluxes \( s \), given measurements \( d \) to satisfy \( d \approx R s \):

- Conventional additive Gaussian error (least-squares): \( d = R s + \xi \)
- Embed probabilistic model for fluxes \( s \): \( d = R (\mu s + C_s \xi) \)
Inferred fluxes show less variability across models.
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LES computation in Scramjet engine: static-vs-dynamic SGS model calibration

Calibrate with Turbulent Kinetic Energy (TKE) data, predict both TKE and Pressure

**TKE**
- **No model error**
- **With model error**

**Pressure**
- **No model error**
- **With model error**