Density Estimation Framework for Model Error Quantification

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Goal: Model Error Quantification

Develop statistical framework for model error representation, quantification and propagation for physical models.

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization
- Inverse modeling context $\quad y_i = f(x_i;\lambda) + \epsilon_i$
- Given data, calibrate for λ, accounting for model error
- Model error is deviation from 'truth'

Truth $g(x) \neq f(x;\lambda)$ Model

Model Error Challenge

Additive model discrepancy (Kennedy-O'Hagan, 2001)

$$y_i = \underbrace{f(x_i;\lambda) + \delta(x_i)}_{\text{truth } g(x_i)} + \epsilon_i$$

has challenges for physical models:

- Strong priors required on $\delta(x)$ to satisfy physical constraints
- Disambiguation of model error $\delta(x_i)$ and data error ϵ_i
- QoI-specific calibration; no extrapolation to other QoIs
- Correlation structure in $\delta(x)$ should ideally be informed by the model $f(x;\lambda)$

Idea: Embedded Model Error

Embed uncertainty within the model

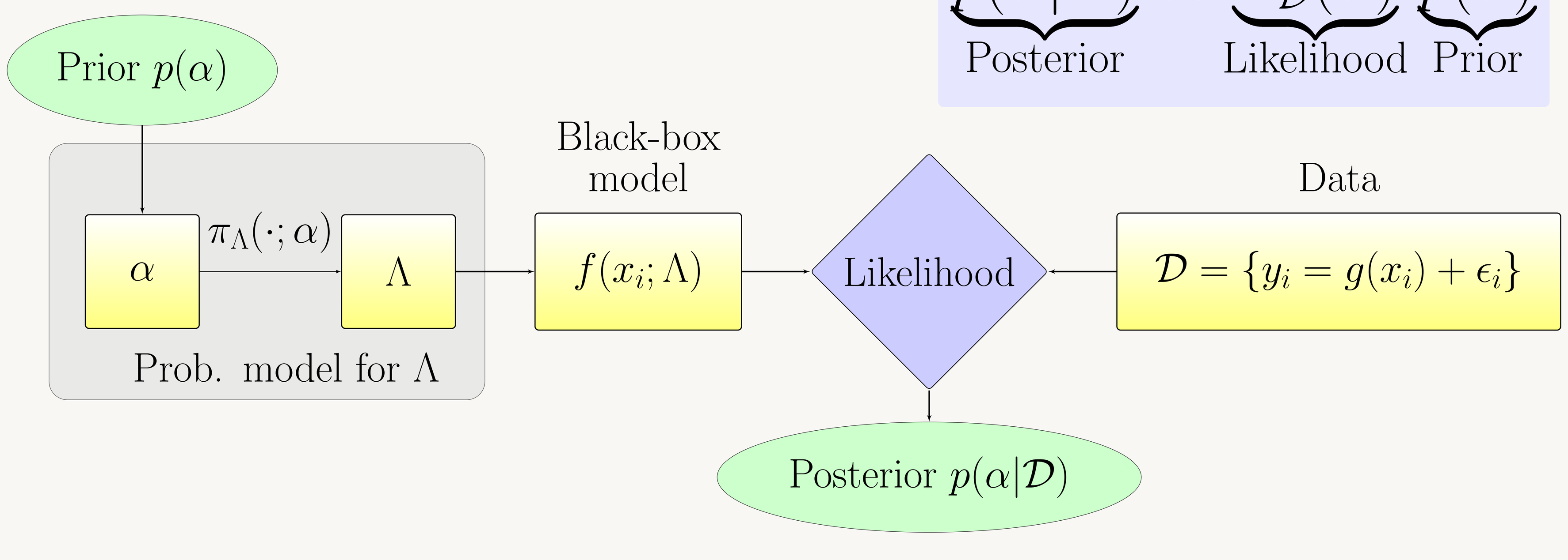
$y_i = f(x_i;\Lambda) + \epsilon_i$	$y_i = f(x_i;\Lambda(x_i)) + \epsilon_i$	$y_i = \tilde{f}(x_i;\lambda,\Theta) + \epsilon_i$
Black-box	*Random field*	*Extra 'physics'*

- Embed model error in specific submodel phenomenology
- Allows targeted model error placement
- Naturally preserves model structure and physical constraints
- Disambiguate model and data errors

- Cast input parameters λ as a random variable Λ
- Parameter estimation of λ turns into PDF estimation of Λ
- Parameterize PDF form $\pi_\Lambda(\cdot;\alpha)$
  - *e.g.* Polynomial Chaos $\Lambda = \sum_{k=0}^{K} \alpha_k \Psi_k(\xi)$
- Back to parameter estimation, now for $\alpha = (\alpha_0, \ldots, \alpha_K)$

Bayesian Density Estimation

$$\underbrace{p(\alpha|\mathcal{D})}_{\text{Posterior}} \propto \underbrace{L_{\mathcal{D}}(\alpha)}_{\text{Likelihood}} \underbrace{p(\alpha)}_{\text{Prior}}$$



K. Sargsyan, H. Najm, and R. Ghanem, "On the Statistical Calibration of Physical Models". *International Journal for Chemical Kinetics*, 47(4): pp 246–276, 2015.

Likelihood Construction

- Full Likelihood: $L(\alpha) = p(y|\alpha) = p(y_1,\ldots,y_N|\alpha) = \pi(y)$
- Marginal Apprx: $L(\alpha) \approx \prod_{i=1}^N p(y_i|\alpha) = \prod_{i=1}^N \pi(y_i)$
- Approximate Bayesian Computation: $L(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(S_M,S_{\mathcal{D}})}{\epsilon}\right)$
- Gaussian Apprx: $L(\alpha) \propto e^{-\frac{1}{2}(y-\mu(\alpha))^T\Sigma^{-1}(\alpha)(y-\mu(\alpha))}$

Forward Prediction

$$f(x;\Lambda) = f\left(x;\sum_k \alpha_k\Psi_k(\xi)\right) \overset{NISP}{=} \sum_k f_k(x;\alpha)\Psi_k(\xi)$$

- Non-intrusive spectral projection (NISP) employed for
  - Likelihood computation and posterior predictions
  - Easy access to first two moments:

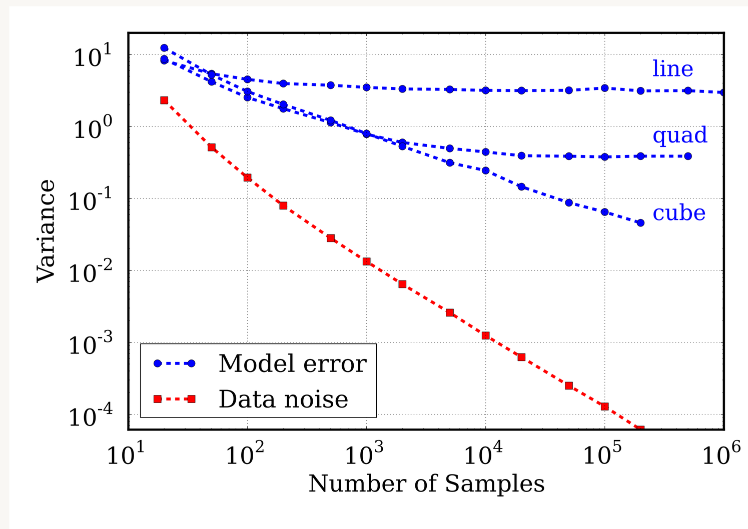
$$\mu(x;\alpha) = f_0(x;\alpha), \qquad \sigma^2(x;\alpha) = \sum_{k>0} f_k^2(x;\alpha)||\Psi_k||^2$$

- Predictive mean $\quad \mathbb{E}[y(x)] = \mathbb{E}_\alpha[\mu(x;\alpha)]$
- Decomposition of predictive variance

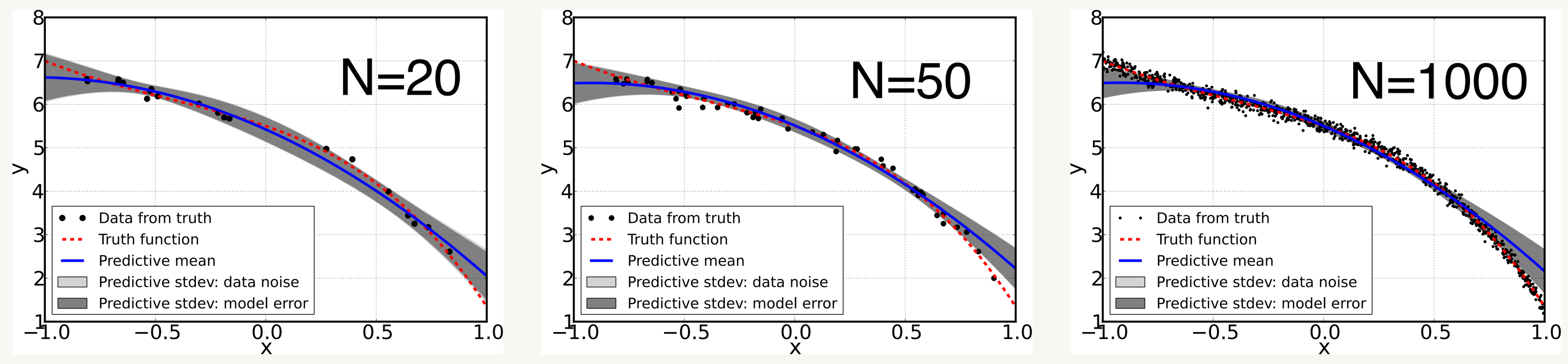
$$\mathbb{V}[y(x)] = \underbrace{\mathbb{E}_\alpha[\sigma^2(x;\alpha)]}_{\text{Model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x;\alpha)] + \sigma_d^2}_{\text{Poserior/Data error}}$$

Demonstration

Calibrating linear, quadratic and cubic models w.r.t. 'truth'
$g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$
measured with noise $\sigma = 0.1$



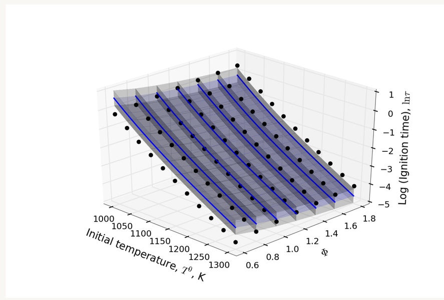
Left-over model error with increased data amount



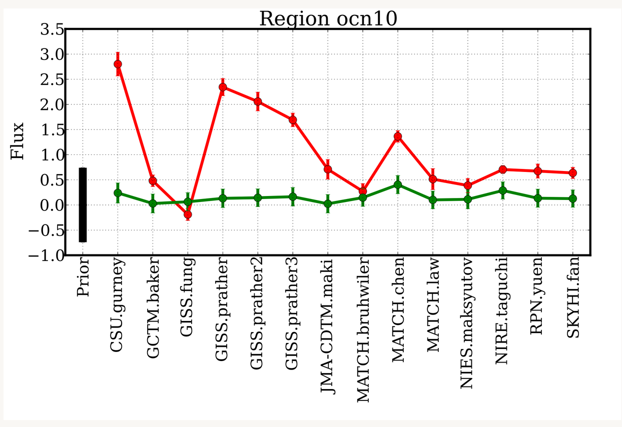
Applications

(1) Chemical ignition of methane: Model-to-model calibration

- Single-step global reaction model calibrated against a detailed chemical kinetic model



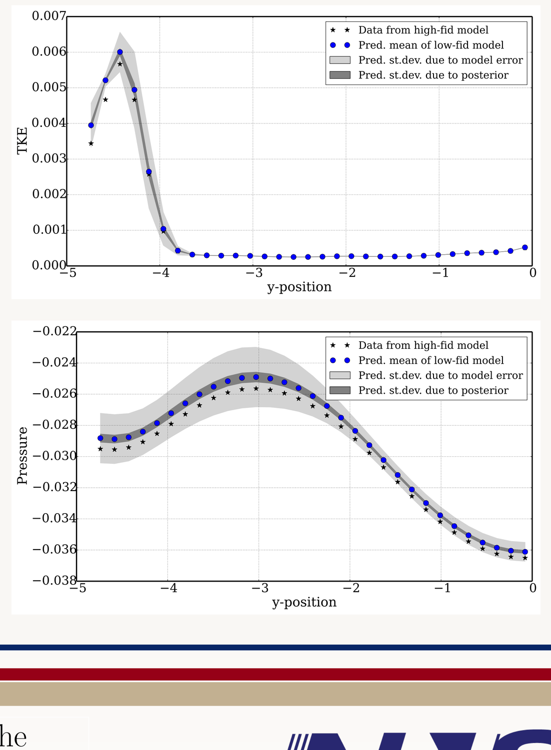
(2) Atmospheric transport: Multi-model calibration



- CO_2 measurements at 77 sites
  - Find fluxes at 22 locations
- Without model error, only 'effective' fluxes are computed

(3) Large eddy simulation of turbulent flow: Extrapolate to other QoIs

- Calibrate static subgrid model vs data from dynamic model
  - Use simulation data of turbulent kinetic energy (TKE), predict both TKE and Pressure



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