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Uncertainty Quantification with model Error

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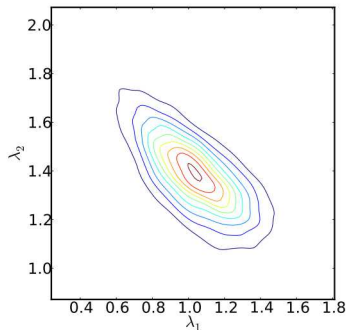
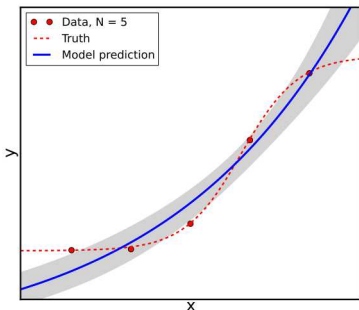
Outline

- 1 Model Error
- 2 Introduction
- 3 Proposed Approach
- 4 Model-to-model Calibration – no data noise
- 5 Chemistry model calibration
- 6 Model calibration with noisy data
- 7 LES with model error
- 8 Closure

Motivation

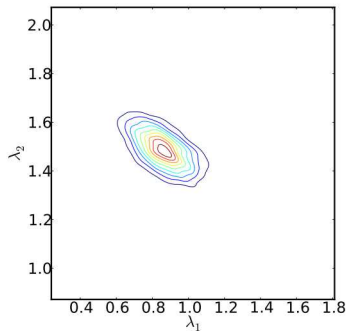
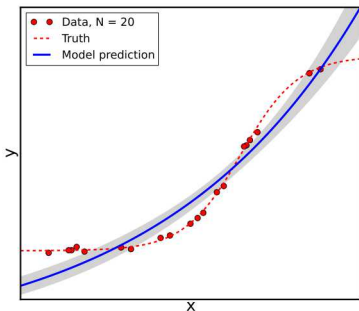
- All models are wrong in principle
- Models of physical systems rely on
 - Presumed theoretical framework
 - Mathematical formulation
- Practical models of complex physical systems rely on
 - Simplifying assumptions
 - Numerical discretization of governing equations
 - Computational software & hardware
- model error is frequently non-negligible
- Estimating model error is useful for
 - model comparison & validation
 - model improvement & scientific discovery
 - reliable computational predictions

Challenges with Model Calibration due to Model Error



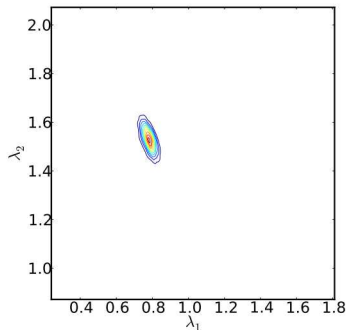
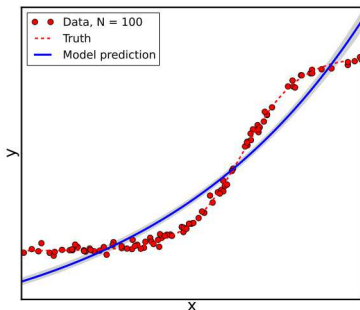
- Conventional parameter estimation context: $y_{\text{data}} = f(x, \lambda) + \epsilon_d$
- Additional data results in reduced parameteric posterior uncertainty
- One gets more confident about predictions with the wrong model
- Predictive uncertainty in calibrated model has no utility for prediction
- Ignoring model error leads to irrelevant predictive errors

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Statistical modeling of model error

Error framework:

Measurements: $y_{\text{data}} = y_{\text{truth}} + \epsilon_d$

Model predictions: $y_{\text{truth}} = y_{\text{model}} + \epsilon_m$

Thus: $y_{\text{data}} = y_{\text{model}} + \epsilon_m + \epsilon_d$

Error modeling - example

Model: $y_{\text{model}} = f(x, \lambda)$

Data Error: $\epsilon_d \sim \mathbf{N}(0, \sigma^2)$

Model Error: $\epsilon_m \sim \mathbf{GP}(\mu(x), C(x, x'))$

Model calibration:

Estimate model parameters λ along with those of ϵ_m, ϵ_d

Kennedy & O'Hagan 2001; Bayarri *et al.* 2002

Challenges – Physical Models

- Arbitrary choice of statistical model (e.g. GP) spatial structure does not take the physical model into acct
 - Potential violation of implicit constraints in physical models
 - e.g. incompressible flow: $\nabla \cdot v = 0$
- Difficulty in disambiguation of model & data error
- Calibration of model error on measured observable does not impact quality of other model predictions

Key idea - Targeted model error embedding

- Embed model error in specific submodel phenomenology (Berliner 2003)
 - a modified transport or constitutive law
 - a modified formulation for a material property
- Pros:
 - 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
 - explore if it can explain discrepancy on observable
 - naturally preserves model structure and associated constraints
- Cons:
 - complex likelihood $p(y|\lambda)$ for general nonlinear $f(x, \lambda, \epsilon_m)$

Consider a simple no-data-noise setting

- Calibration of a (simple) model against a complex model
- Let the complex model be presumed to represent the truth
- In this context, the data has no noise
- Discrepancy between model and data is all due to model error

$$y_{\text{data}} = y_{\text{truth}} = y_{\text{complex_model}} = y_{\text{model}} + \epsilon_m$$

- $\epsilon_m = y_{\text{data}} - y_{\text{model}}$ is a deterministic quantity
- The only information as to the quality of the calibrated uncertain model, e.g. via a posterior predictive check, is in a unique ϵ_m for any x

model-to-model calibration

Model: $y = f(x, \lambda, \phi(\epsilon_m))$

- Random variable ϕ in augmented model components carries model error

Data: $D = \{(x_i, y_{\text{data},i}), i = 1, \dots, N\}$

- Goal:
 - Establish $\lambda, p(\phi)$ such that the likelihood of the data is high, based on the posterior predictive $p(y|D)$
- This puts us in a density estimation framework for ϕ :
 - The utility of additional data is to improve the specification of λ , and $p(\phi)$

Present Context

Embed ϵ_m in λ

- In other words: $\lambda \leftarrow \lambda + \epsilon_m$
- Model: $y = f(x, \lambda)$ with $\lambda : \Omega \rightarrow \mathbb{R}^M$
- Density estimation problem for $p(\lambda)$
- λ : a random field $\lambda(x, \omega)$, or a random variable $\lambda(\omega)$
 - focus on the latter
- Let the random variable λ be parameterized by α
 - For example, define λ as a polynomial chaos expansion

$$\lambda = \sum_{k=0}^P \alpha_k \Psi_k(\xi)$$

- Parameter estimation problem for $\alpha = (\alpha_0, \dots, \alpha_P)$
- Bayesian setting
 - Prior $\pi(\alpha)$
 - Likelihood $L(\alpha) = p(D|\alpha)$

Full Likelihood

$$L(\alpha) = p(D|\alpha) = \pi_f(y_{\text{data},1}, \dots, y_{\text{data},N}|\alpha)$$

where:

$\pi_f(\cdot|\alpha)$: N -variate density of the random variable (f_1, \dots, f_N)
 with $f_i = f(x_i, \lambda(\xi; \alpha))$

Problem: $\pi_f(\cdot)$ is degenerate in general when $N > M$

- Consider a case with $M = 1$, $\lambda \sim N(\mu, \sigma^2)$, and $f = \lambda$
- Let $N = 2$, hence $(f_1, f_2) = (\lambda, \lambda)$ for any λ sample
- With $f_1 = f_2 = \lambda$, (f_1, f_2) are dependent and $\pi_f(\cdot|\mu, \sigma)$ is non-zero only along the line $f_2 = f_1$
- $\pi_f(y_{\text{data},1}, y_{\text{data},2}|\mu, \sigma)$ is non-zero only along the line $y_{\text{data},2} = y_{\text{data},1}$
 \Rightarrow potentially can ameliorate singularity with a smoothing nugget

Marginalized Likelihood

$$L(\alpha) = p(D|\alpha) = \prod_{i=1}^N \pi_{f_i}(y_{\text{data},i}|\alpha)$$

where

$\pi_{f_i}(\cdot, \alpha)$ is the univariate density of the RV $f_i = f(x_i, \lambda(\alpha))$

Problem: the likelihood has multiple singularities corresponding to α values leading to vanishing marginal variances at each x_i

- Gaussian example: Let $f_i \sim \mathcal{N}(\mu_i(\alpha), \sigma_i(\alpha)^2)$, then

$$L(\alpha) = \frac{1}{(2\pi)^{N/2}} \prod_{i=1}^N \frac{1}{\sigma_i(\alpha)} \exp\left(-\frac{(\mu_i(\alpha) - y_{\text{data},i})^2}{2\sigma_i(\alpha)^2}\right)$$

- Multiple singularities, $\sigma_i(\alpha) = 0, i = 1, \dots, N$
- Posterior maximization always finds one of these singularities, fitting one point perfectly, while misfitting the rest

\Rightarrow can potentially be controlled via priors on α

Approximate Bayesian Computation (ABC)

Employ a kernel density as a pseudo-likelihood to enforce select constraints:

Uncertain prediction $p(y|D)$ is centered on the data

- With $\mu_i(\alpha) = \mathbb{E}_\xi[f(x_i, \lambda(\xi; \alpha))]$:
minimize $\| \mu_i(\alpha) - y_{\text{data},i} \|$

The width of the distribution $p(y|D)$ is consistent with the spread of the data around the nominal model prediction

- With $\sigma_i^2(\alpha) = \mathbb{V}_\xi[f(x_i, \lambda(\xi, \alpha))]$:
minimize $\| \sigma_i(\alpha) - \gamma |\mu_i(\alpha) - y_{\text{data},i}| \|$
- γ is a factor that specifies the desired match between σ_i and the discrepancy $|\mu_i(\alpha) - y_{\text{data},i}|$, on average

ABC Likelihood

With $\rho(\mathcal{S})$ being a metric of the statistic \mathcal{S} , use the kernel function as an ABC likelihood:

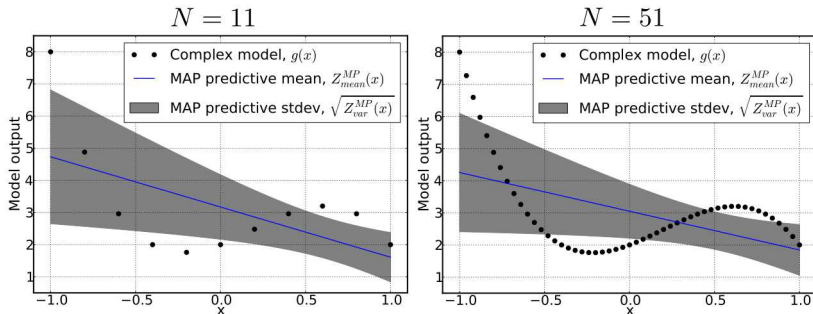
$$L_{\text{ABC}}(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S})}{\epsilon}\right)$$

where ϵ controls the severity of the consistency control

Propose the Gaussian kernel density:

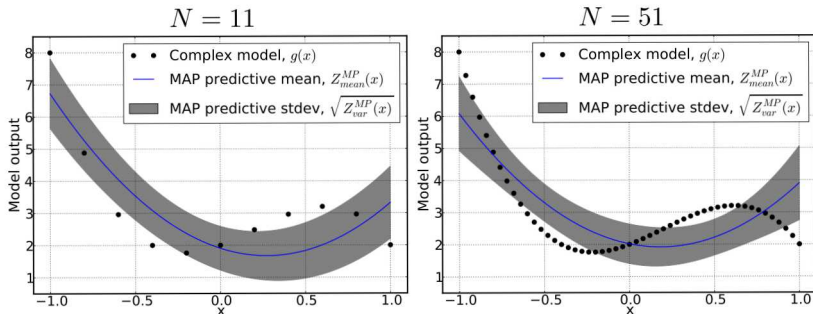
$$L_{\epsilon}(\alpha) = \frac{1}{\epsilon\sqrt{2\pi}} \prod_{i=1}^N \exp\left(-\frac{(\mu_i(\alpha) - y_{d,i})^2 + (\sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{d,i}|)^2}{2\epsilon^2}\right)$$

Test problem – Cubic data fit by a line – ABC



- MAP predictive (MP) mean centered on data
- MP standard deviation captures range of discrepancy
- Increasing number of data points has a small effect on both MP mean and stdev

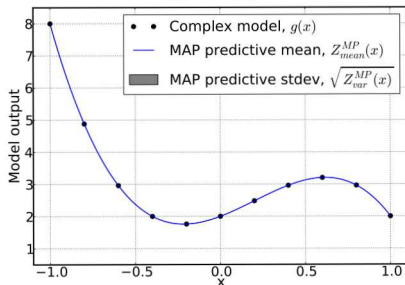
Test problem – Cubic data fit by a quadratic – ABC



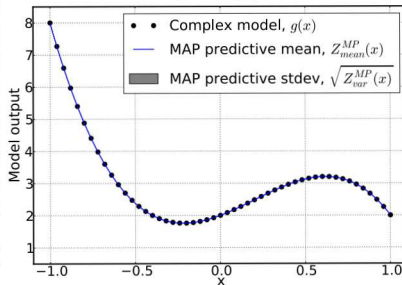
- Quadratic has better fit to the data
- Smaller MP stdev consistent with smaller discrepancy

Test problem – Cubic data fit by a cubic – ABC

$N = 11$



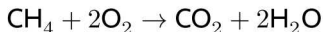
$N = 51$



- Cubic has perfect fit to the data
- Negligible MP stdev consistent with negligible discrepancy

Chemistry problem – ABC

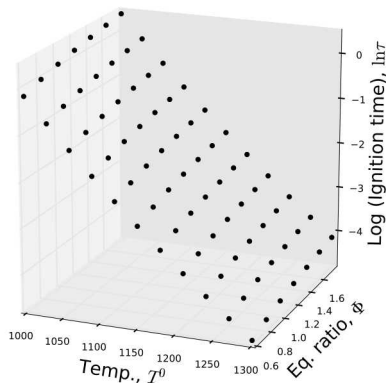
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model – ODE system
- Data: ignition time; range of initial T & equivalence ratio
- Single-step model:



$$\mathfrak{R} = [\text{CH}_4][\text{O}_2]k$$

$$k = A \exp(-E/R^o T)$$

$$\lambda = \begin{bmatrix} \ln A \\ E \end{bmatrix} = \sum_{k=0}^P \alpha_k \Psi_k(\xi)$$



Constant Pressure Ignition – Problem Structure

- N species, M reactions, rate parameter vector λ
- State vector $u = (X_1, \dots, X_N, T)$ – mole fractions, temperature
- ODE system

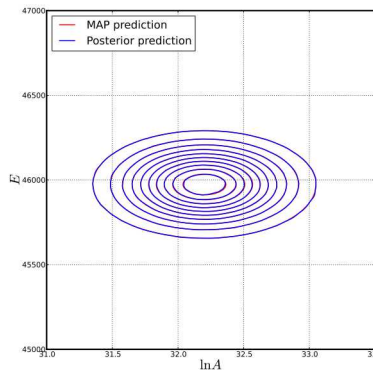
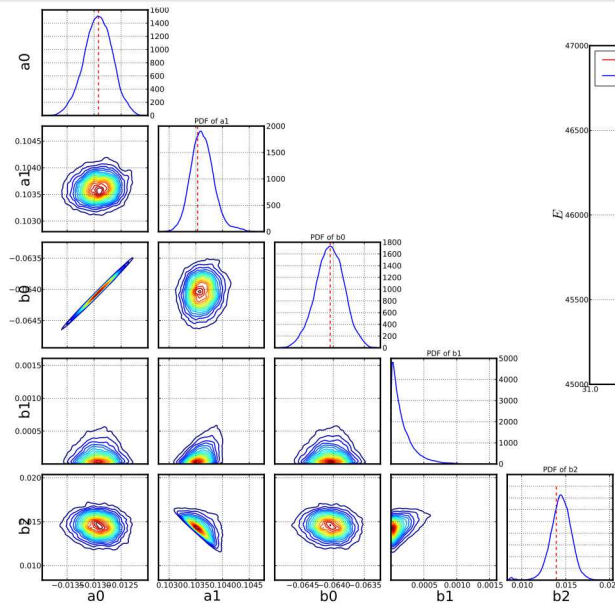
$$\begin{aligned}\frac{du_i(t; \lambda)}{dt} &= w_i(u; \lambda), \quad i = 1, \dots, N \\ u(0) &= u_0\end{aligned}$$

- Observable: ignition time $\tau_{\text{ign}}(u_0, \lambda) = t |_{T(t; u_0, \lambda) = T_{\text{ign}}}$
- Challenge, for any proposed λ , computing $\tau_{\text{ign}}(u_0, \lambda)$ is expensive
 - Large stiff ODE system for complex fuels
- Polynomial chaos formulation allows construction of a surrogate

$$\tau_{\text{ign}}(u_0, \lambda(\xi; \alpha)) = f(u_0, \xi; \alpha) = \sum_{k=0}^P f_k(u_0; \alpha) \Psi_k(\xi)$$

- Surrogate replaces the forward model in the Likelihood function

Posterior on α – Posterior Predictive on $(\ln A, E)$

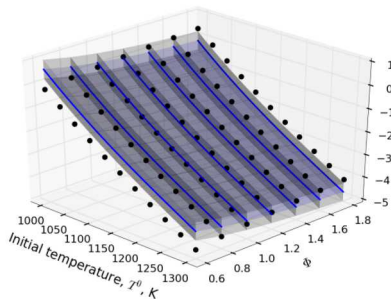


Quality of Uncertain Calibrated Model Predictions

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

Over the range of (T^0, Φ) :

- MAP predictive mean ignition-time is centered on the data
- MAP predictive stdv is consistent with the scatter of the data



Consider a noisy-data setting

- Calibration of a model $y_m = f(x, \lambda)$ against noisy data
- Synthetic noisy data is generated from a “truth” model + Gaussian noise
- Discrepancy between fit model prediction and data is due to both model error & data noise

$$y = y_{\text{data}} = y_{\text{truth}} + \epsilon = f(x, \lambda) + \epsilon$$

- Modeling strategy:
 - Model λ as a random vector, represented with PC
 - Represent the noise similarly using PC
 - Estimate all PC coefficients using Bayesian inference

Model Error formulation – noisy data

$$y = f(x, \lambda) + \epsilon$$

Let $\epsilon \sim N(0, \sigma^2)$. With *N.i.i.d.* data points we have

$$y_i = f(x_i, \lambda) + \epsilon_i, \quad i = 1, \dots, N$$

For Hermite-Gaussian PC:

$$\begin{aligned} \lambda &= \sum_{k=0}^P \alpha_k \Psi_k(\xi_1, \dots, \xi_d), & \alpha &\equiv (\alpha_0, \dots, \alpha_P) \\ f(x, \lambda) &= \sum_{k=0}^P f_k(x, \alpha) \Psi_k(\xi_1, \dots, \xi_d) \\ y_i &= \sum_{k=0}^P f_k(x_i, \alpha) \Psi_k(\xi_1, \dots, \xi_d) + \sigma \xi_{d+i} \end{aligned}$$

Augmented PC germ $\xi = (\underbrace{\xi_1, \dots, \xi_d}_{\epsilon_m}, \underbrace{\xi_{d+1}, \dots, \xi_{d+N}}_{\epsilon_d})$

Model Error Estimation – noisy data

Inverse problem:

- Given:
 - data:

$$D = \{(x_i, y_i)\}_{i=1}^N$$

- data model:

$$y_i = \underbrace{\sum_k f_k(x_i, \alpha) \Psi_k(\xi_1, \dots, \xi_d)}_{y_{\text{model}}(\epsilon_m)} + \underbrace{\sigma \xi_{d+i}}_{\epsilon_d}, \quad i = 1, \dots, N$$

- Estimate parameters (α, σ)

Bayesian context:

- posterior: $p(\alpha, \sigma | D)$
- options: Full Bayesian likelihood; Marginalized; ABC
- All are viable here in principle, as the data noise introduces regularity
- We illustrate the case with a Marginalized Gaussian approximation

Calibrated Uncertain Model Posterior Predictive

- Calibrated data model : $y_i = f(x_i; \lambda(\xi; \alpha)) + \sigma \xi_{d+i}$
- Full posterior on α, σ : $\alpha, \sigma \sim p(\alpha, \sigma | D)$
- Marginal posteriors: $\alpha \sim p(\alpha | D), \sigma \sim p(\sigma | D)$
- Posterior Predictive (PP):

$$p(y|D) = \int p(y|\alpha, \sigma) p(\alpha, \sigma | D) d\alpha d\sigma = \mathbb{E}_{\alpha, \sigma} [p(y|\alpha, \sigma)]$$

- PP Mean :

$$\mathbb{E}_{\text{PP}}[y] = \mathbb{E}_{\alpha} [\mathbb{E}_{\xi}[f]]$$

- PP Variance:

$$\mathbb{V}_{\text{PP}}[y] = \underbrace{\mathbb{E}_{\alpha} [\mathbb{V}_{\xi}[f]]}_{\text{model error}} + \underbrace{\mathbb{E}_{\sigma} [\sigma^2] + \mathbb{V}_{\alpha} [\mathbb{E}_{\xi}[f]]}_{\text{data noise}}$$

Calibrated Uncertain Model Predictions

- Calibrated model : $y = f(x; \lambda(\xi; \alpha))$
- Marginal posterior on α : $\alpha \sim p(\alpha|D)$
- Pushed forward posterior (PFP):

$$p(f|D) = \int p(f|\alpha)p(\alpha|D)d\alpha = \mathbb{E}_{\alpha}[p(f|\alpha)]$$

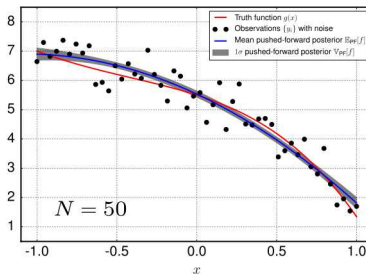
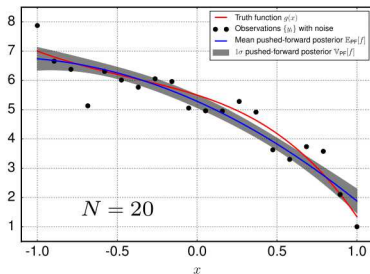
- PFP Mean :

$$\mathbb{E}_{\text{PFP}}[f] = \mathbb{E}_{\alpha}[\mathbb{E}_{\xi}[f]]$$

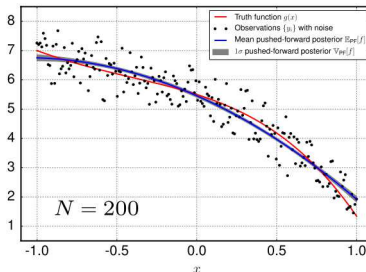
- PFP Variance:

$$\mathbb{V}_{\text{PFP}}[f] = \underbrace{\mathbb{E}_{\alpha}[\mathbb{V}_{\xi}[f]]}_{\text{model error}} + \underbrace{\mathbb{V}_{\alpha}[\mathbb{E}_{\xi}[f]]}_{\text{data noise}}$$

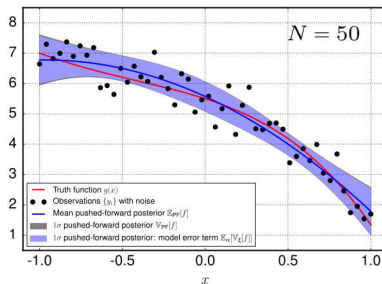
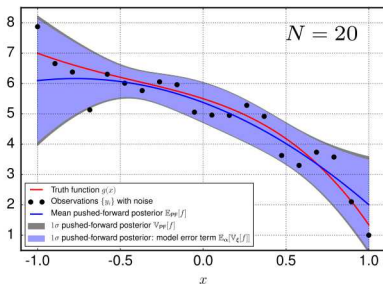
Quadratic-fit – Classical Bayesian likelihood



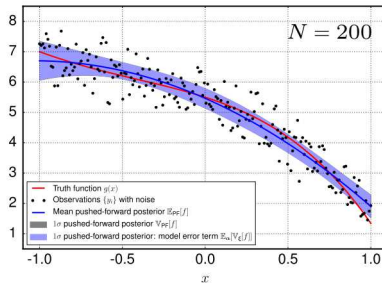
- With additional data, predictive uncertainty around the wrong model is indefinitely reducible
- Predictive uncertainty not indicative of discrepancy from truth



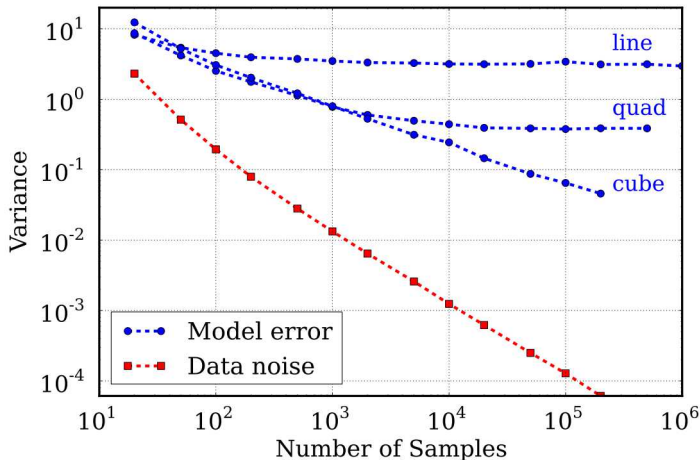
Quadratic-fit – ModErr – MargGauss



- With additional data, predictive uncertainty due to data noise is reducible
- Predictive uncertainty due to model error is not reducible



Model Error – Fit with Different Models



LES subgrid static-vs-dynamic – Jet-in-crossflow

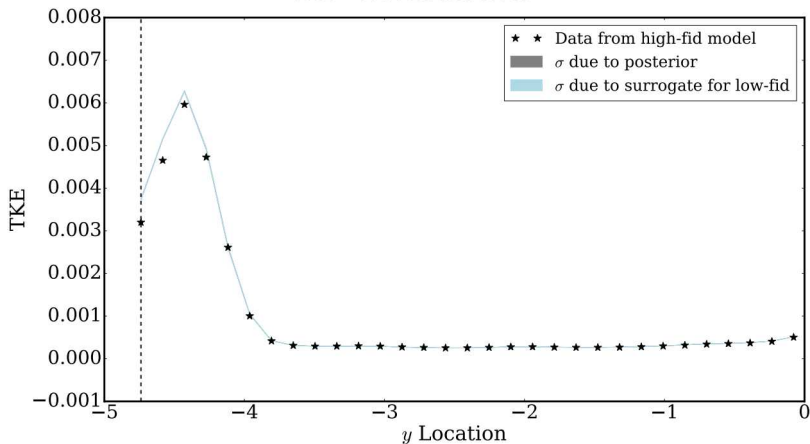
- Large Eddy Simulation (LES) subgrid model fidelity
 - Dynamic: subgrid parameters variable in space/time, g_i
 - Static : subgrid parameters constant in space/time, $f_i(\lambda)$
- Target: Calibrate a static model against a dynamic model
 - Fit parameters $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1})$ of static model $f(\lambda)$ to data from dynamic model simulations, accounting for model error
- Static model surrogate construction using $4^3 = 64$ simulations of $f(\lambda)$
 - Legendre polynomial expansion surrogate of 3-rd order
 - Account for surrogate error: *i.i.d.* zero-bias Gaussian noise
 - Global sensitivity analysis: impact of $C_R \gg$ impact of Pr_t^{-1} and Sc_t^{-1}
 - Selected only C_R for model error embedding

$$\mathbb{V}_{\text{PPF}}[f] = \underbrace{\mathbb{E}_{\alpha}[\mathbb{V}_{\xi}[f]]}_{\text{model error}} + \underbrace{\mathbb{V}_{\alpha}[\mathbb{E}_{\xi}[f]]}_{\alpha \text{ posterior}} + \underbrace{\mathbb{E}_{\sigma_S}[\sigma_S^2]}_{\text{surrogate error}}$$

Calibrate with TKE data; Predict both TKE and Pressure

Pushed forward posterior

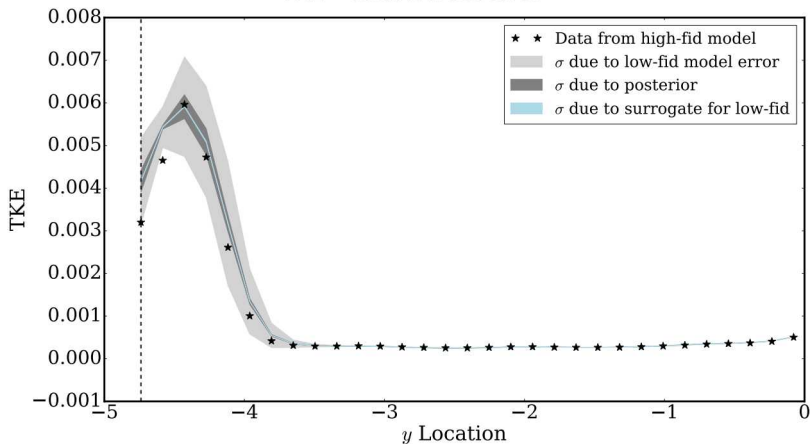
TKE - No model error



Calibrate with TKE data; Predict both TKE and Pressure

Pushed forward posterior

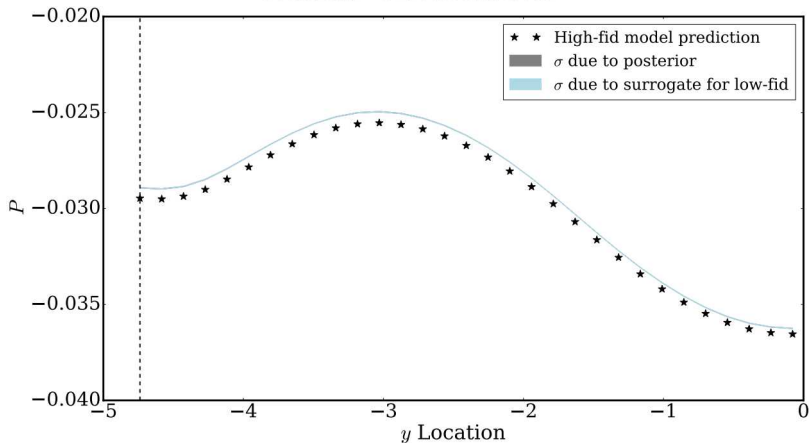
TKE - With model error



Calibrate with TKE data; Predict both TKE and Pressure

Pushed forward posterior

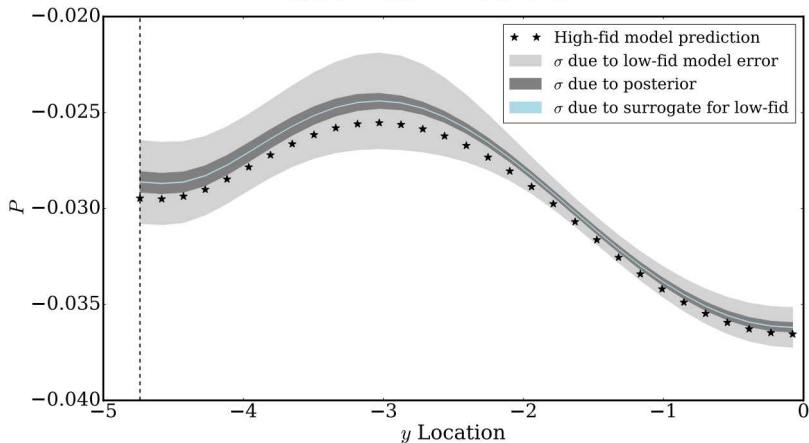
Pressure – No model error



Calibrate with TKE data; Predict both TKE and Pressure

Pushed forward posterior

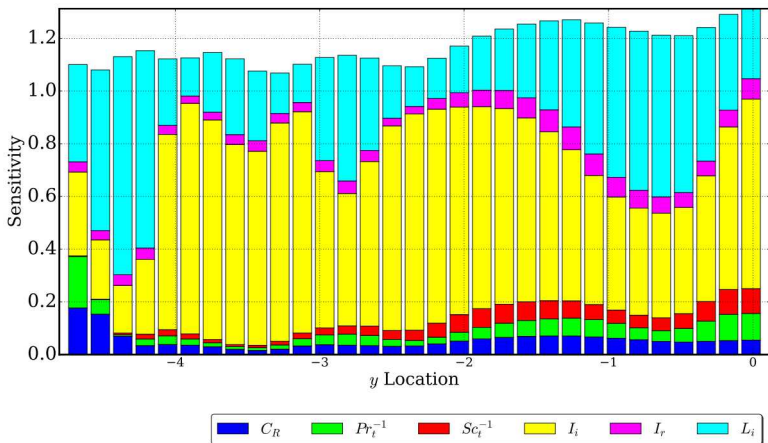
Pressure – With model error



LES subgrid 2D-vs-3D – Jet-in-crossflow

- Target: Calibrate a 2D LES model against a 3D model
 - Fit parameters $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1}, I_i, I_r, L_i)$ of 2D model to data from 3D model simulations, accounting for model error
 - Parameters:
 - C_R : Smagorinsky constant
 - Pr_t : Turbulent Prandtl number
 - Sc_t : Turbulent Schmidt number
 - I_i : Turb. intensity (inflow air) horizontal component
 - I_r : Turb. intensity (inflow air) ratio: vertical/horizontal
 - L_i : Length scale of most energetic eddies
- 2D model surrogate construction
 - Account for surrogate error: *i.i.d.* zero-bias Gaussian noise
 - Global sensitivity analysis
 - Selected one parameter (I_i) for model error embedding
 - Calibrate 2D model with observable: Mach no. $M(y)$ at a given x -location
 - Predict both $M(y)$ and pressure $P(y)$, and compare to 3D model

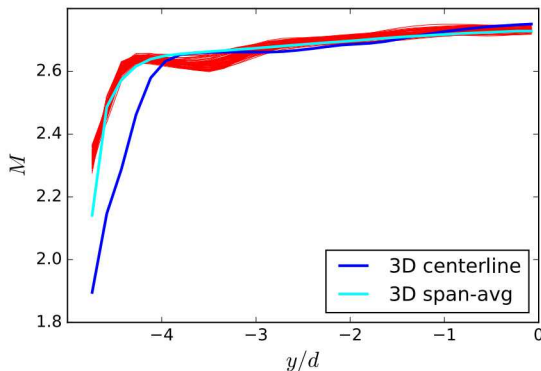
Global Sensitivity Analysis Results



Dominant paramter is I_i : employ it to embed model error

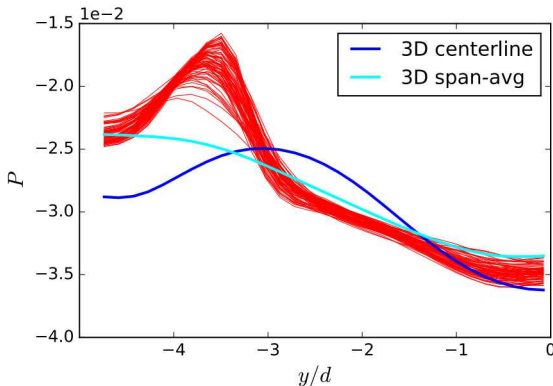
Model Error – Case study: 2D-vs-3D

- Problem Focus: P1 Jet in Crossflow problem
 - static SGS constants, $d/8$ grid resolution
- Calibrate a 2D model using 3D benchmark simulations as data
- Quantify the model error associated with 2D treatment
- Red curves show ensemble of 2D runs over λ -range
- 3D QoI selection for 2D comparison: (a) centerline, (b) spanwise average



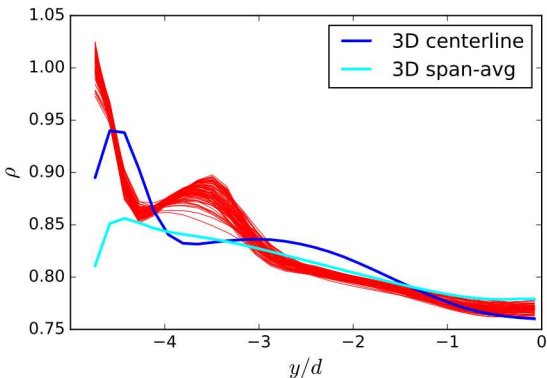
Model Error – Case study: 2D-vs-3D

- Problem Focus: P1 Jet in Crossflow problem
 - static SGS constants, $d/8$ grid resolution
- Calibrate a 2D model using 3D benchmark simulations as data
- Quantify the model error associated with 2D treatment
- Red curves show ensemble of 2D runs over λ -range
- 3D QoI selection for 2D comparison: (a) centerline, (b) spanwise average



Model Error – Case study: 2D-vs-3D

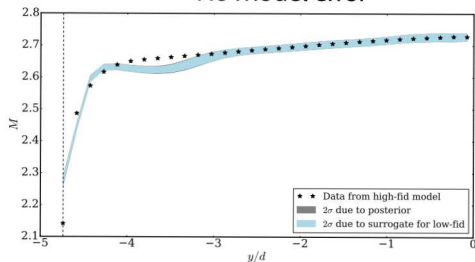
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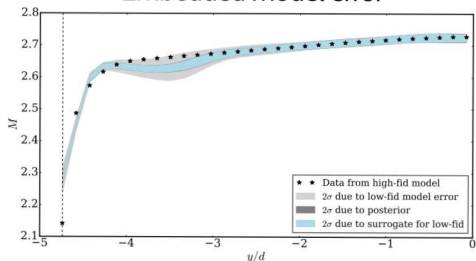
Model Error – Mach Number spanwise-average

- Model error contribution captures the discrepancy

No model error



Embedded model error

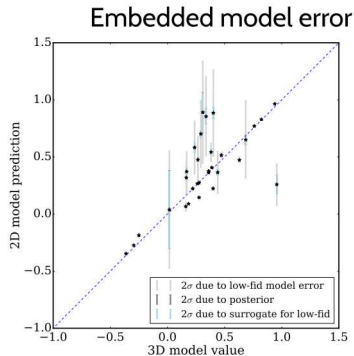
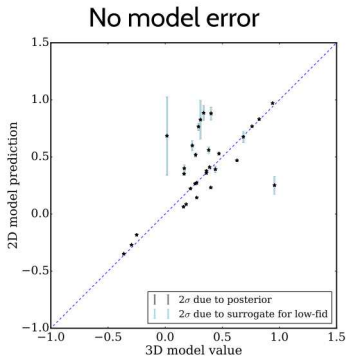


$$\sigma_i^2 = \underbrace{\mathbb{E}_{\tilde{\lambda}} [\sigma_i^2(\tilde{\lambda})]}_{\text{Model error}} + \underbrace{\mathbb{V}_{\tilde{\lambda}} [\mu_i(\tilde{\lambda})]}_{\text{Posterior uncertainty}} + \underbrace{(\sigma_i^{LOO})^2}_{\text{Surrogate error}}$$



Model Error – Select Qols

- Model error contribution captures the discrepancy for averaged quantities across a wide range of observables



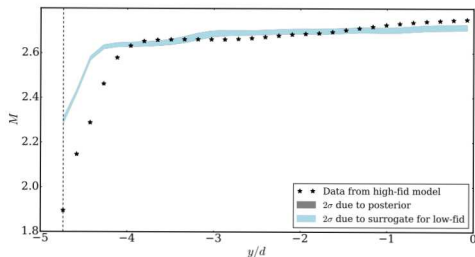
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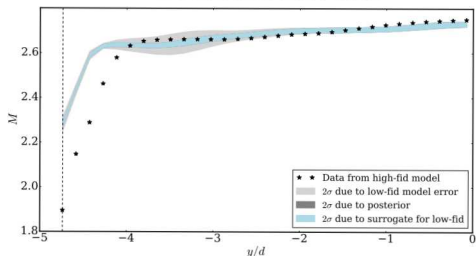
Model Error – Mach Number centerline

- Model error contribution extends as much as prior allows

No model error



Embedded model error



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Closure

- Presented a strategy for dealing with model error
 - targeted at physical models
- Density estimation framework – $y = f(x; \lambda(\xi; \alpha))$
- Uncertain predictions with the calibrated model include uncertainty due to both model-error and data-noise
- Results suggest disambiguation of the two components
- Demonstrations in chemical ignition and LES of jet-in-crossflow
 - Including accounting for PC surrogate error
- Limitation of model-error embedding: when no variation of the chosen parameter in the simple model could reproduce results of the detailed model
 - Expand parameter prior range(s)
 - Consider other parameters
 - Propose a modification in the model