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Uncertainty Quantification with Model Error

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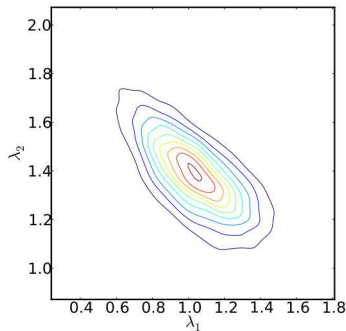
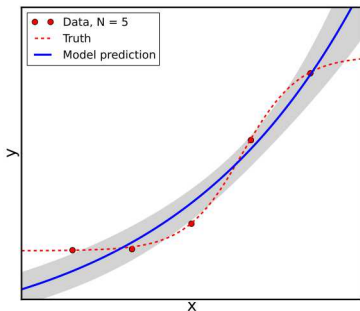
Outline

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

Motivation

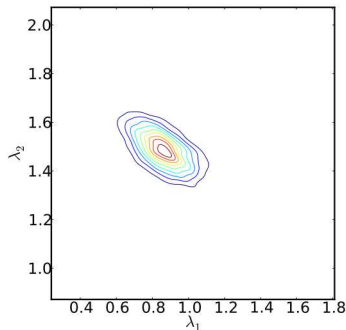
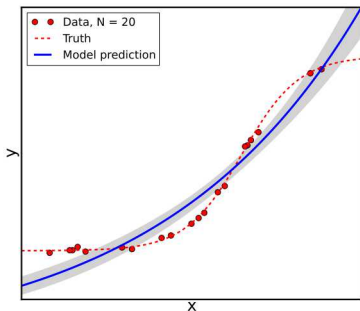
- All models are wrong in principle
- Models of physical systems rely on
 - Presumed theoretical framework
 - Mathematical formulation
- Practical models of complex physical systems rely on
 - Simplifying assumptions
 - Numerical discretization of governing equations
 - Computational software & hardware
- 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



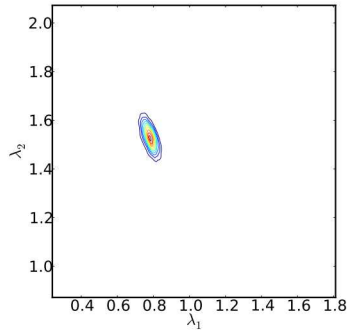
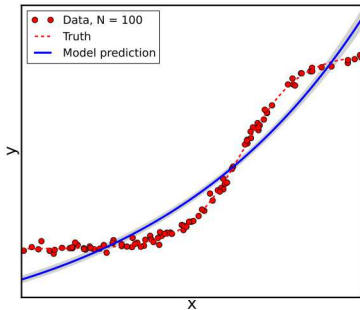
- Conventional parameter estimation context: $y_{\text{data}} = f(x, \lambda) + \epsilon_d$
- Additional data results in reduced parameteric posterior uncertainty
- One gets more confident about predictions with the wrong model
- Predictive uncertainty in calibrated model has no utility for prediction
- 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
- Physical scientists are unlikely to augment their model with a statistical model error term on select outputs

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 $L(\alpha) = p(D|\alpha)$

Polynomial Chaos Expansion (PCE)

- Given a *germ* $\xi(\omega) = \{\xi_1, \dots, \xi_n\}$ – a set of *i.i.d.* RVs
 - where $p(\xi)$ is uniquely determined by its moments

Any RV in $L^2(\Omega, \mathfrak{G}(\xi), P)$ can be written as a PCE:

$$u(\omega) = f(\xi) = \sum_{k=0}^{\infty} u_k \Psi_k(\xi(\omega))$$

- u_k are mode strengths
- $\Psi_k()$ are functions orthogonal w.r.t. $p(\xi)$

Orthogonal basis examples:

- Hermite polynomials with Gaussian germ
- Legendre polynomials with Uniform germ, ...
- Global versus Local PC methods
 - Adaptive domain decomposition of the support of ξ

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:

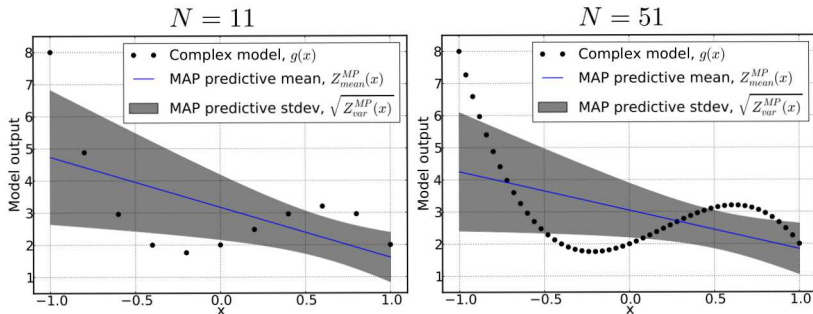
$$L_{\text{ABC}}(\alpha) = \frac{1}{\epsilon} K \left(\frac{\rho(\mathcal{S})}{\epsilon} \right)$$

where ϵ controls the severity of the consistency control

Propose the Gaussian kernel density:

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

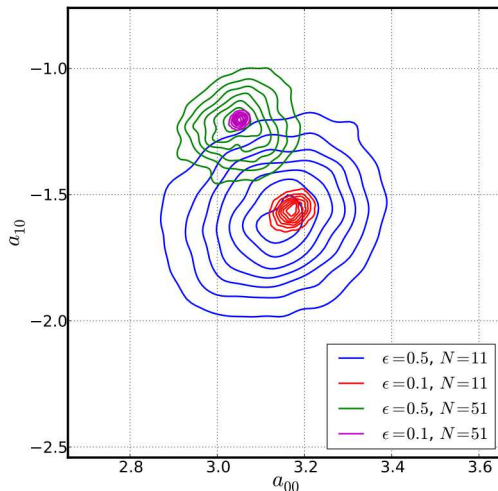
Test problem – Cubic data fit by a line – ABC



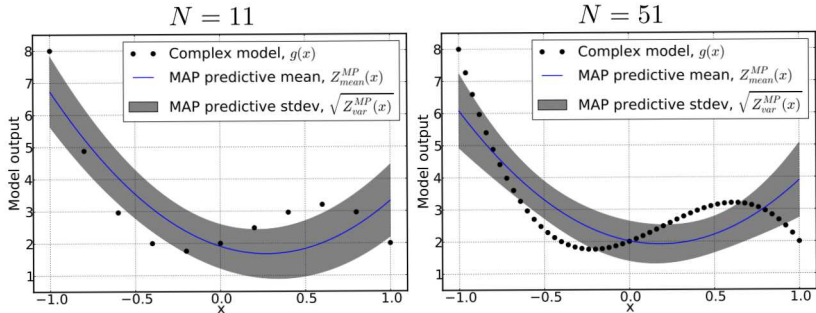
- MAP predictive (MP) mean centered on data
- MP standard deviation captures range of discrepancy
- Increasing number of data points has a small effect on both MP mean and stdev

Test problem – Posterior density on α

- Cubic data, line-fit
- Joint posterior on two elements of α
- Uncertainty in α is decreased by
 - Increasing N
 - Decreasing ϵ

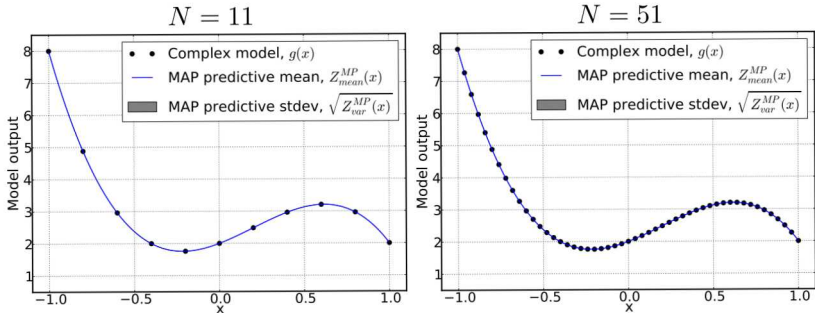


Test problem – Cubic data fit by a quadratic – ABC



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

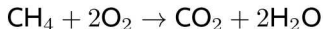
Test problem – Cubic data fit by a cubic – ABC



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

Chemistry problem – ABC

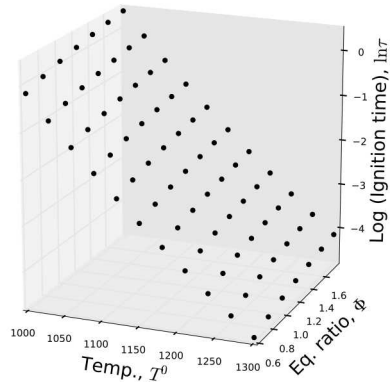
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model – ODE system
- Data: ignition time; range of initial T & equivalence ratio
- Single-step model:



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

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

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



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

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

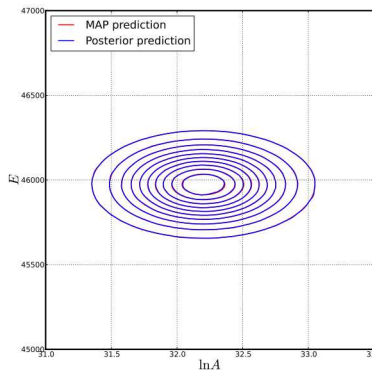
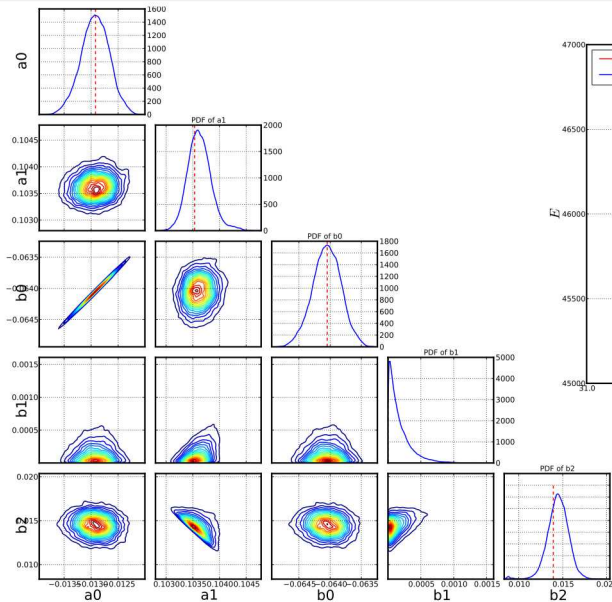
- Observable: ignition time $\tau_{\text{ign}}(u_0, \lambda) = t |_{T(t; u_0, \lambda) = T_{\text{ign}}}$
- Challenge, for any proposed λ , computing $\tau_{\text{ign}}(u_0, \lambda)$ is expensive
 - Large stiff ODE system for complex fuels
- Polynomial chaos formulation allows construction of a surrogate

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

- Surrogate replaces the forward model in the Likelihood function

Posterior on α

-

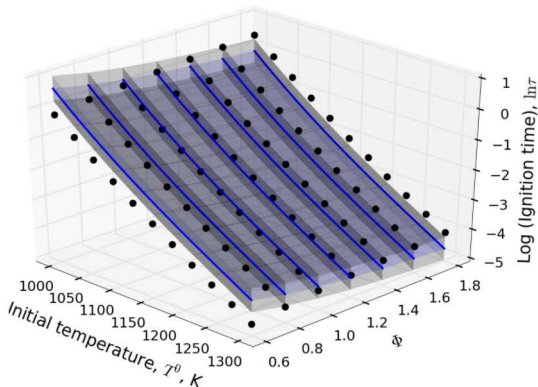
Posterior Predictive on $(\ln A, E)$ 

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

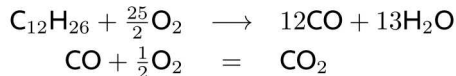


K. Sargsyan, HNN, and R. Ghanem
 "On the Statistical Calibration of Physical Models"
 Int. J. Chem. Kin., 47(4): 246-276, 2015

n -dodecane ignition – 1

with L. Hakim, M. Khalil, J. Oefelein, and G. Lacaze, SNL

- Homogeneous ignition, n -dodecane/air mixture
- Two-step global reaction model calibrated against a “detailed” model
 - Reference chemical kinetic model: 255 species, 2289 reactions
Narayanaswamy *et al.* 2014
- Data: ignition time; range of initial T & equivalence ratio Φ
- Two-step model:



$$\mathfrak{R}_1 = Ae^{\frac{-E}{RT}} [\text{C}_{12}\text{H}_{26}]^{0.25} [\text{O}_2]^{1.25}$$

$$\mathfrak{R}_{2f} = 3.98 \cdot 10^{14} e^{\frac{-4 \cdot 10^4}{RT}} [\text{CO}] [\text{H}_2\text{O}]^{0.5} [\text{O}_2]^{0.25}$$

$$\mathfrak{R}_{2b} = 5 \cdot 10^8 e^{\frac{-4 \cdot 10^4}{RT}} [\text{CO}_2]$$

- $E = \lambda_0, \quad \ln A = \lambda_1 + \lambda_2 e^{\lambda_3 \Phi} + \lambda_4 \tanh((\lambda_5 + \lambda_6 \Phi)T_0) + \lambda_7$

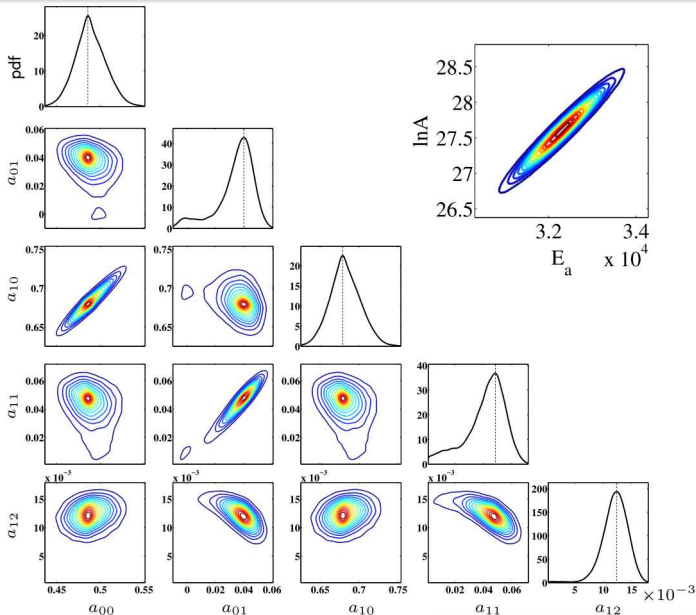
n -dodecane ignition – 2

- $(E, \ln A) = (\lambda_0, \lambda_1 + \lambda_2 e^{\lambda_3 \Phi} + \lambda_4 \tanh((\lambda_5 + \lambda_6 \Phi)T_0 + \lambda_7))$
- Original parameter vector $\lambda = (\lambda_0, \dots, \lambda_7)$
- Embed model error in (λ_0, λ_1)
- PCE model:

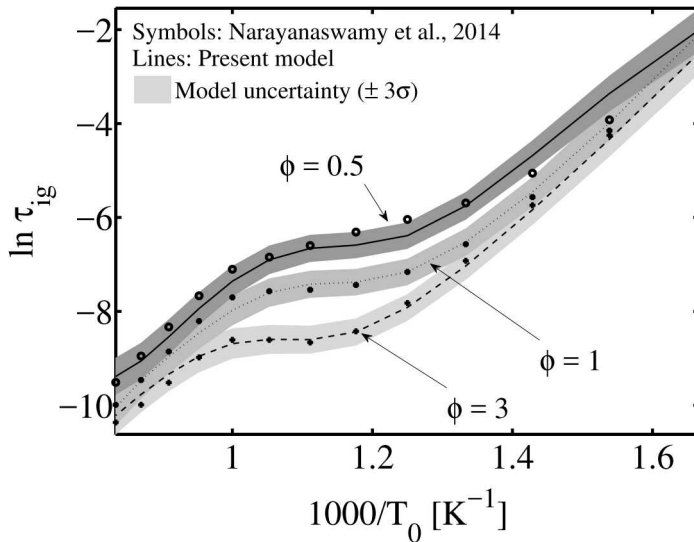
$$\begin{aligned}\lambda_0 &= a_{00} + a_{01}\xi_1 \\ \lambda_1 &= a_{10} + a_{11}\xi_1 + a_{12}\xi_2 \\ \lambda_2 &= a_{20} \\ &\vdots \\ \lambda_7 &= a_{70}\end{aligned}$$

- ABC targets parameters $(a_{00}, a_{01}, a_{10}, a_{11}, a_{12}, a_{20}, \dots, a_{70})$

n -dodecane ignition – 3



n -dodecane ignition – 4



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:

$$\lambda = \sum_{k=0}^P \alpha_k \Psi_k(\xi_1, \dots, \xi_d), \quad \alpha \equiv (\alpha_0, \dots, \alpha_P)$$

$$f(x, \lambda) = \sum_{k=0}^P f_k(x, \alpha) \Psi_k(\xi_1, \dots, \xi_d)$$

$$y_i = \sum_{k=0}^P f_k(x_i, \alpha) \Psi_k(\xi_1, \dots, \xi_d) + \sigma \xi_{d+i}$$

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):

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

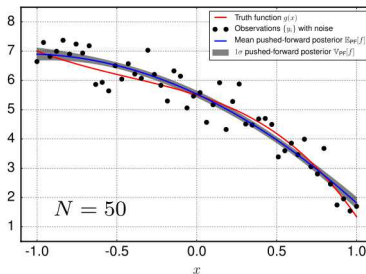
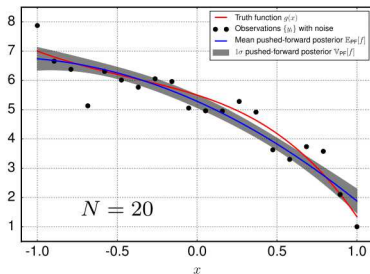
- PFP Mean :

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

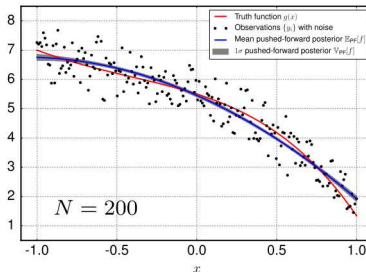
- PFP Variance:

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

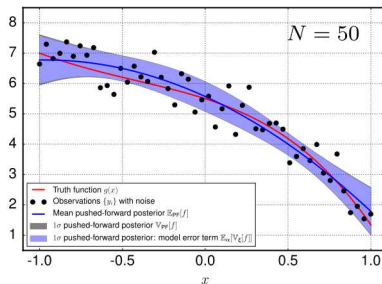
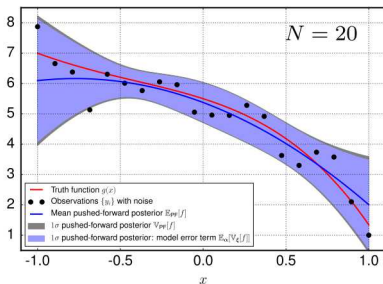
Quadratic-fit – Classical Bayesian likelihood



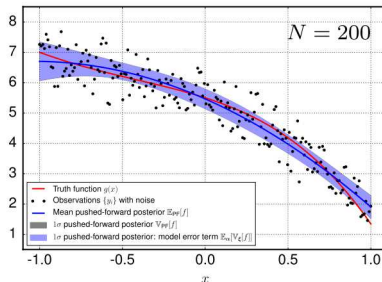
- With additional data, predictive uncertainty around the wrong model is indefinitely reducible
- Predictive uncertainty not indicative of discrepancy from truth



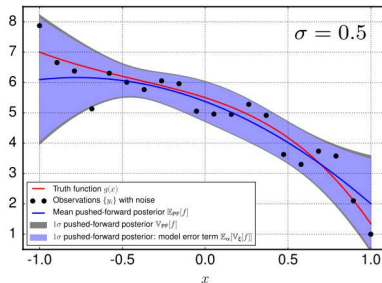
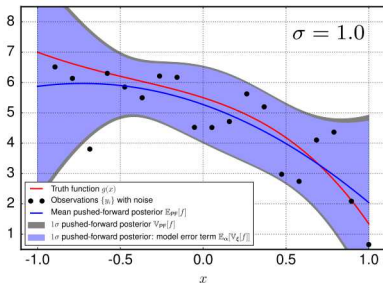
Quadratic-fit – ModErr – MargGauss



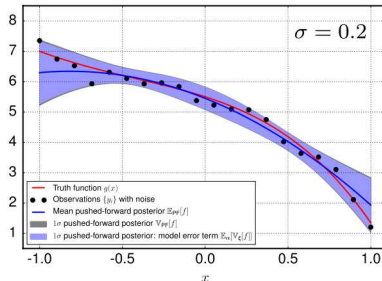
- With additional data, predictive uncertainty due to data noise is reducible
- Predictive uncertainty due to model error is not reducible



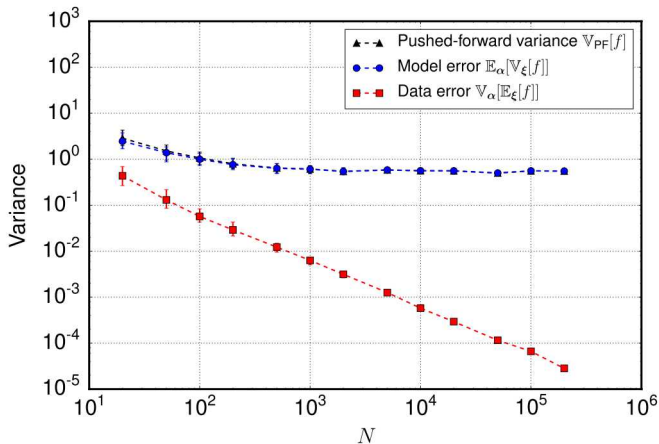
Quadratic-fit – ModErr – MargGauss



- Predictive uncertainty composed of both model-error and data-noise components
- The data-noise component is reducible with lower-noise in the data

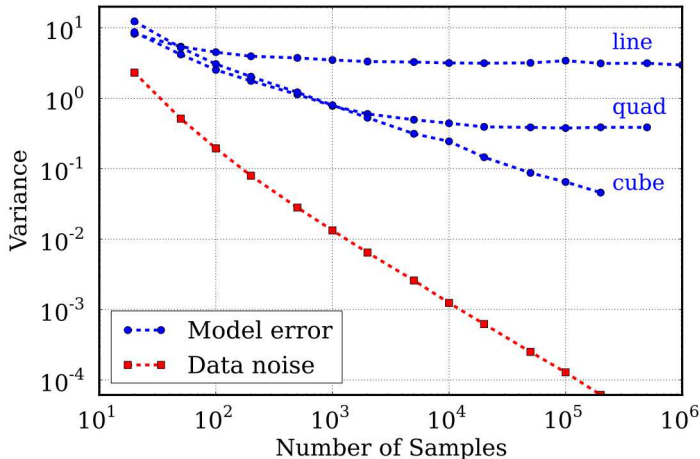


Quadratic-fit – ModErr – MargGauss



Calibrating a quadratic $f(x)$ w.r.t. $g(x) = 6 + x^2 + 0.5(x + 1)^{3.5}$

Model Error – Fit with Different Models



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

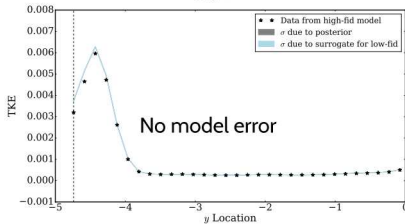
- Large Eddy Simulation (LES) subgrid model fidelity
 - Dynamic: subgrid parameters variable in space/time, g_i
 - Static : subgrid parameters constant in space/time, $f_i(\lambda)$
- Target: Calibrate a static model against a dynamic model
 - Fit parameters $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1})$ of 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

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

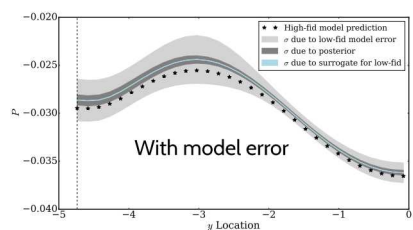
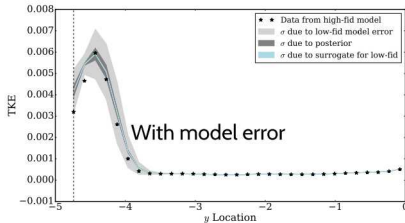
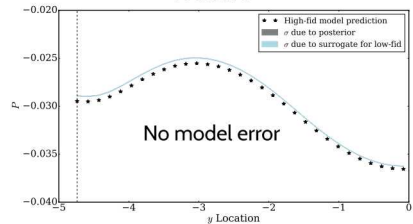
Calibrate with TKE data; Predict both TKE and Pressure

Pushed forward posterior

TKE



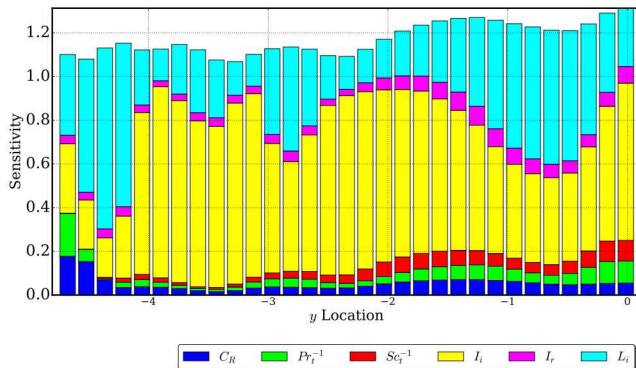
Pressure



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

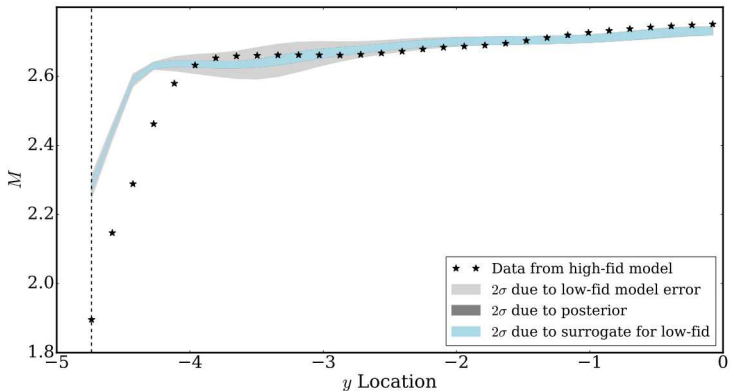
- Target: Calibrate a 2D LES model against a 3D model
 - Fit parameters $\lambda = (C_R, Pr_t^{-1}, Sc_t^{-1}, I_i, I_r, L_i)$ of 2D model to data from 3D model simulations, accounting for model error
- 2D model surrogate construction
 - Account for surrogate error: *i.i.d.* zero-bias Gaussian noise
 - Global sensitivity analysis
 - Selected one parameter for model error embedding
 - Calibrate 2D model with observable: $M(y)$ at a given x -location
 - Predict both $M(y)$ and $P(y)$, and compare to 3D model

Global Sensitivity Analysis Results



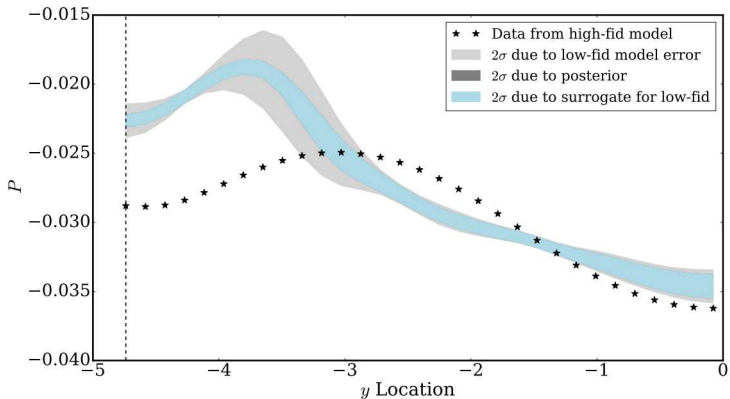
- Dominant paramter is I_i : employ it to embed model error

Posterior Predictive on Calibration QoI: M



- Poor 2D model performance in the near-wall region
- Insufficient correction via embedded model error

Posterior Predictive on another QoI: P



- Worse 2D model, including model error, performance for prediction of pressure
- No variation in I_r is sufficient to explain the discrepancy between 2D and 3D models

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