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On Model Error and Statistical Calibration of Physical Models

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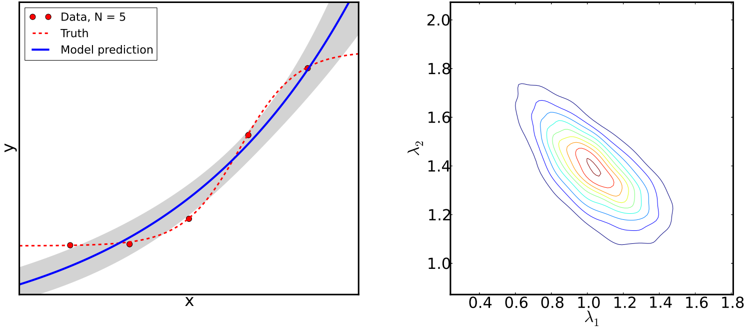
Outline

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: $y_{\text{data}} = f(x, \lambda) + \epsilon_{\text{d}}$
- 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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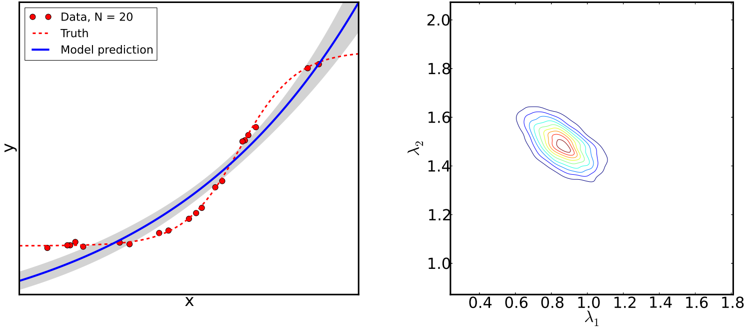

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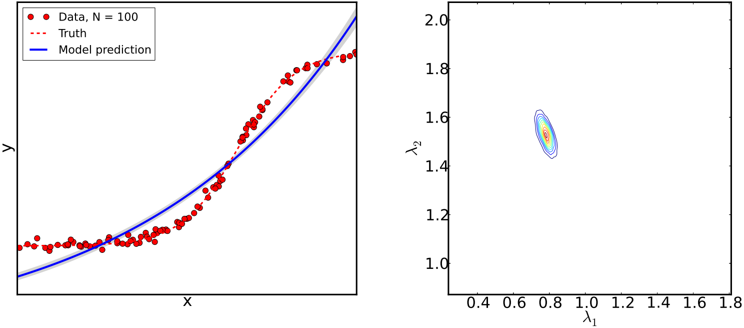

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Statistical modeling of model error

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: $$\epsilon_d \sim \text{N}(0, \sigma^2)$$

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

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

- Goal:
  - Establish λ, $p(\phi)$ 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

- Model: $y = f(x, \lambda)$ with $\lambda : \Omega \to \mathbb{R}^M$
- 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 $\alpha = (\alpha_0, \cdots, \alpha_P)$
- Bayesian setting
  - Prior $\pi(\alpha)$
  - Likelihood $L(\alpha) = p(D|\alpha)$

Polynomial Chaos Expansion (PCE)

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

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

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

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

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 $\boldsymbol{\xi}$

Full Likelihood

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

where:

$\pi_f(\cdot|\alpha)$: N-variate density of the random variable $(f_1, \ldots, f_N)$
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 $f_i \sim \mathsf{N}(\mu_i(\alpha), \sigma_i(\alpha)^2)$, 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, $\sigma_i(\alpha) = 0$, $i = 1, \ldots, N$
- 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 $\mu_i(\alpha) = \mathsf{E}_\xi[f(x_i, \lambda(\xi;\alpha))]$:

$$\text{minimize} \parallel \mu_i(\alpha) - y_{\text{data},i} \parallel$$

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

- With $\sigma_i^2(\alpha) = \mathsf{V}_\xi[f(x_i, \lambda(\xi,\alpha))]$:

$$\text{minimize} \parallel \sigma_i(\alpha) - \gamma|\mu_i(\alpha) - y_{\text{data},i}| \parallel$$

- 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:

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

where ϵ controls the severity of the consistency control

Propose the Gaussian kernel density:

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

Likelihood construction – variants/approxmiations

- Full Likelihood

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

- Marginalized Likelihood

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

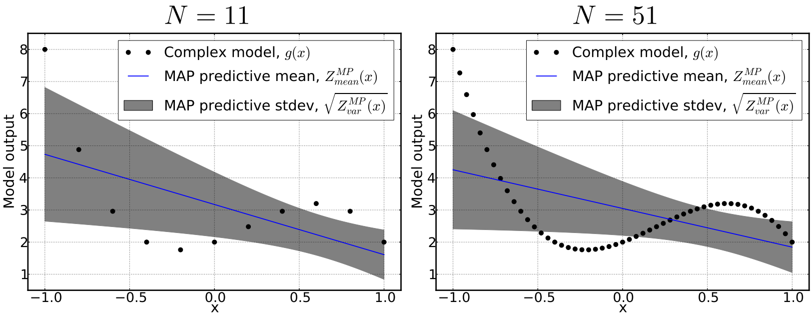
- Approximate Bayesian Computation:
  Seek to satisfy the constraints:
  - $p(y|D)$ is "centered" on the data
  - The width of the distribution $p(y|D)$ is "consistent" with the spread of the data around the nominal model prediction

Prediction

$$
\begin{aligned}
p(\alpha|D) &= p(\alpha_0, \dots, \alpha_P|D) \\
\lambda(\xi;\alpha) &= \sum_{k=0}^{P} \alpha_k \Psi_k(\xi) \\
Z(x,\xi;\alpha) &= f(x, \lambda(\xi;\alpha))
\end{aligned}
$$

MAP predictive RV	$Z^{\text{MP}}(x)$	$= Z(x;\alpha_{\text{MAP}})$
MAP predictive mean	$Z^{\text{MP}}_{\text{mean}}(x)$	$= \mathbb{E}_\xi[Z|\alpha_{\text{MAP}}]$
MAP predictive variance	$Z^{\text{MP}}_{\text{var}}(x)$	$= \mathbb{V}_\xi[Z|\alpha_{\text{MAP}}]$

Test problem – Cubic data fit by a line – ABC

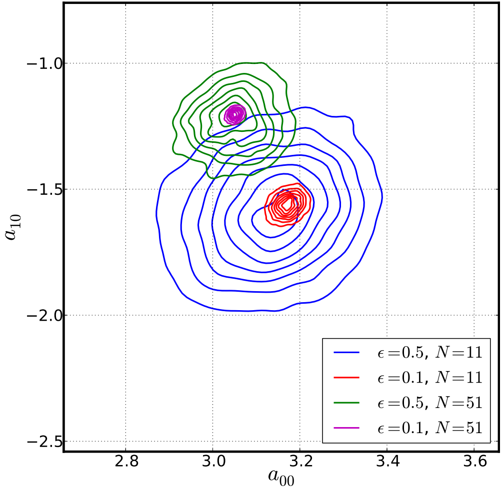


- MAP predictive (MP) mean centered on data
- MP standard deviation captures range of discrepancy
- Increasing number of data points has a small effect on both MP mean and stdev

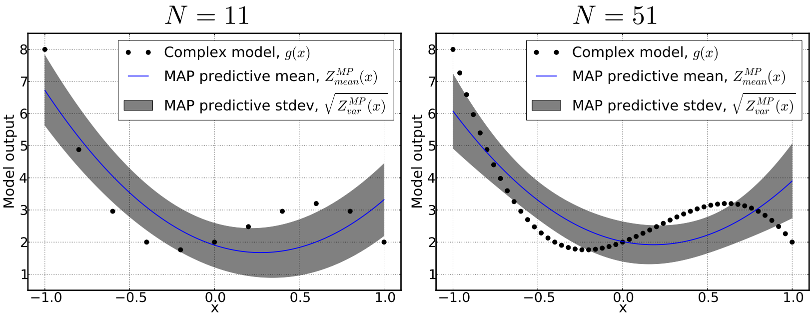
Test problem – Posterior density on α

- Cubic data, line-fit
- Joint posterior on two elements of α

- Uncertainty in α is decreased by
  - Increasing N
  - Decreasing ϵ

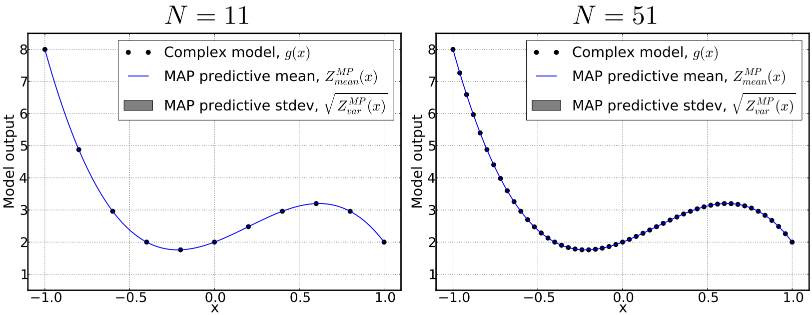


Test problem – Cubic data fit by a quadratic – ABC



- 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

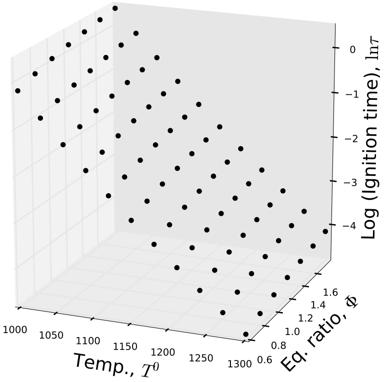
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model – ODE system
- Data: ignition time; range of initial T & equivalence ratio
- Single-step model:

$$\mathrm{CH_4} + 2\mathrm{O_2} \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O}$$

$$\mathfrak{R} = [\mathrm{CH_4}][\mathrm{O_2}]k$$

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

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



Constant Pressure Ignition – Problem Structure

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

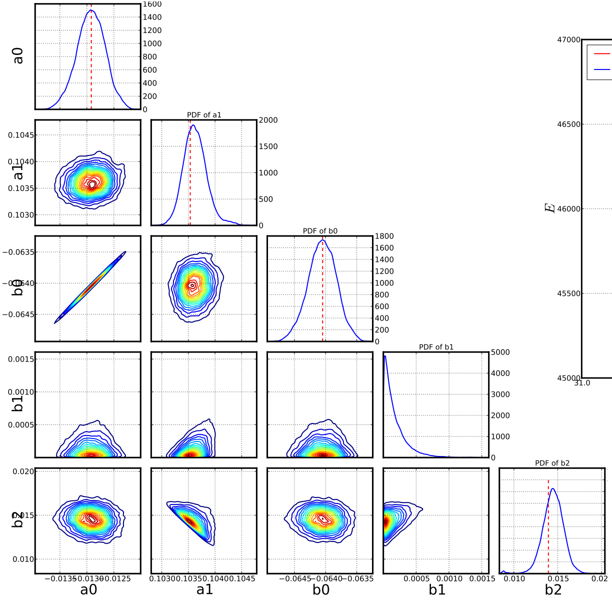
$$\begin{aligned}\frac{\mathrm{d}u_i(t;\lambda)}{\mathrm{d}t} &= w_i(u;\lambda), \quad i = 1, \ldots, N \\ u(0) &= u_0\end{aligned}$$

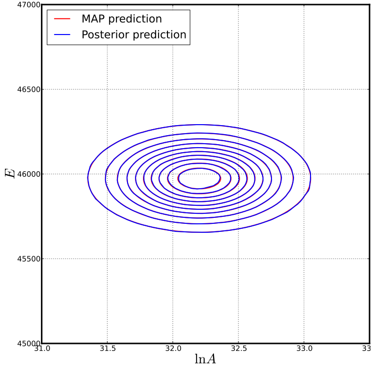
- Observable: ignition time $\tau_{\text{ign}}(u_0, \lambda) = t\,|_{T(t;u_0,\lambda)=T_{\text{ign}}}$
- Challenge, for any proposed λ, computing $\tau_{\text{ign}}(u_0, \lambda)$ is expensive
  - Large stiff ODE system for complex fuels
- Polynomial chaos formulation allows construction of a surrogate

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

- Surrogate replaces the forward model in the Likelihood function

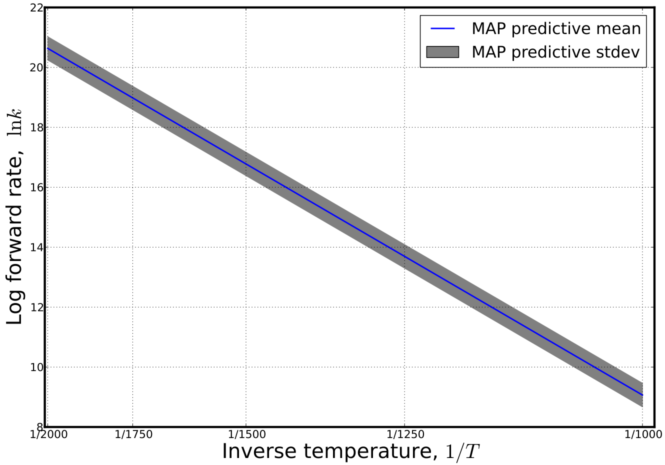
Posterior on α – Posterior Predictive on $(\ln A, E)$





Posterior predictive distribution on ln k

$$\mathsf{E}_\alpha[p(\ln k|D)]$$

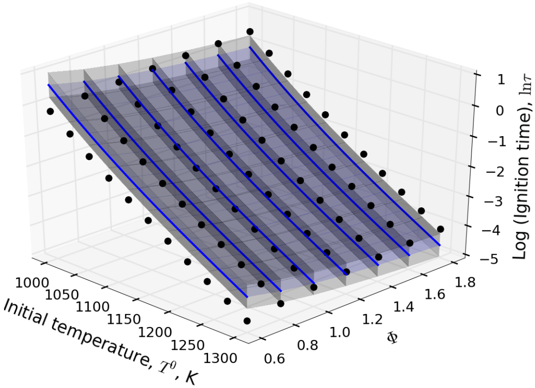


Quality of Uncertain Calibrated Model Predictions

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:

$$\begin{aligned} \mathrm{C_{12}H_{26}} + \tfrac{25}{2}\mathrm{O_2} &\longrightarrow 12\mathrm{CO} + 13\mathrm{H_2O} \\ \mathrm{CO} + \tfrac{1}{2}\mathrm{O_2} &= \mathrm{CO_2} \end{aligned}$$

$$\begin{aligned} \mathfrak{R}_1 &= A e^{\frac{-E}{RT}} [\mathrm{C_{12}H_{26}}]^{0.25} [\mathrm{O_2}]^{1.25} \\ \mathfrak{R}_{2f} &= 3.98 \cdot 10^{14} e^{\frac{-4 \cdot 10^4}{RT}} [\mathrm{CO}][\mathrm{H_2O}]^{0.5} [\mathrm{O_2}]^{0.25} \\ \mathfrak{R}_{2b} &= 5 \cdot 10^{8} e^{\frac{-4 \cdot 10^4}{RT}} [\mathrm{CO_2}] \end{aligned}$$

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

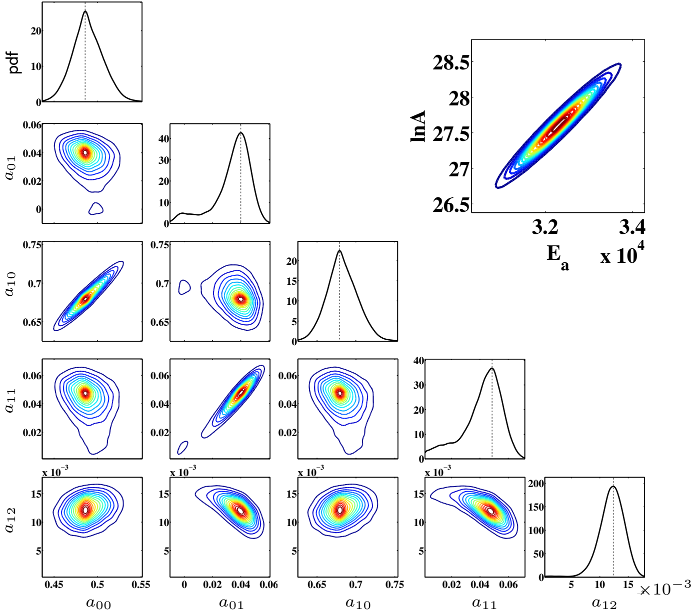
n-dodecane ignition – 2

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

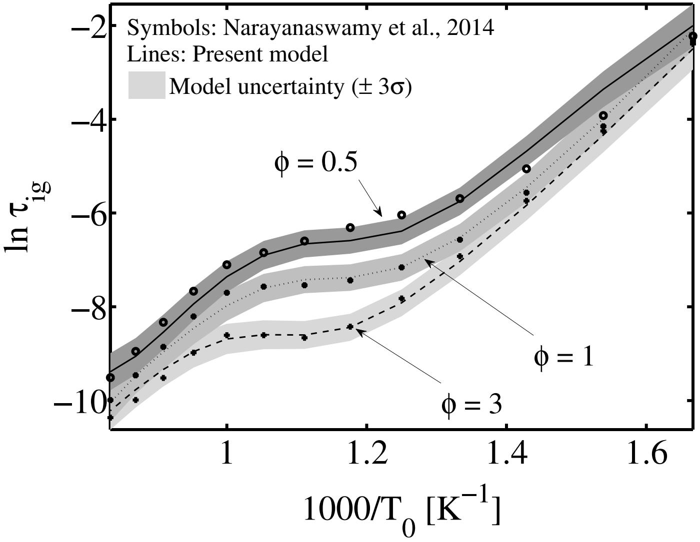
$$\begin{aligned} \lambda_0 &= a_{00} + a_{01}\xi_1 \\ \lambda_1 &= a_{10} + a_{11}\xi_1 + a_{12}\xi_2 \\ \lambda_2 &= a_{20} \\ &\vdots \\ \lambda_7 &= a_{70} \end{aligned}$$

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

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

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

For Hermite-Gaussian PC:

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

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

Model Error Estimation – noisy data

Inverse problem:

- Given:
  - data:

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

  - data model:

$$y_i = \underbrace{\sum_k f_k(x_i, \alpha)\Psi_k(\xi_1, \cdots, \xi_d)}_{y_{\mathrm{model}}(\epsilon_{\mathrm{m}})} + \underbrace{\sigma\, \xi_{d+i}}_{\epsilon_{\mathrm{d}}}, \qquad i = 1, \ldots, N$$

- 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):

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

- 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):

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

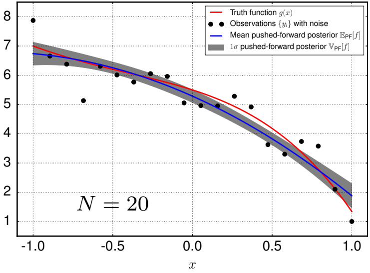
- PFP Mean :

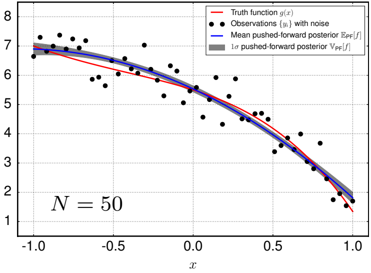
$$\mathbb{E}_{\text{PFP}}[f] = \mathbb{E}_\alpha[\mathbb{E}_\xi[f]]$$

- PFP Variance:

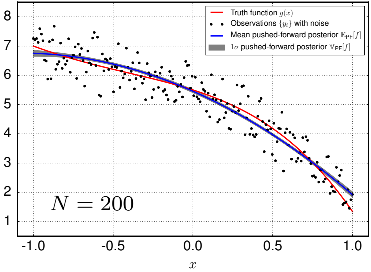
$$\mathbb{V}_{\text{PFP}}[f] = \underbrace{\mathbb{E}_\alpha[\ \mathbb{V}_\xi[\ f\ ]\ ]}_{\text{model error}} + \underbrace{\mathbb{V}_\alpha[\ \mathbb{E}_\xi[\ f\ ]\ ]}_{\text{data noise}}$$

Quadratic-fit – Classical Bayesian likelihood

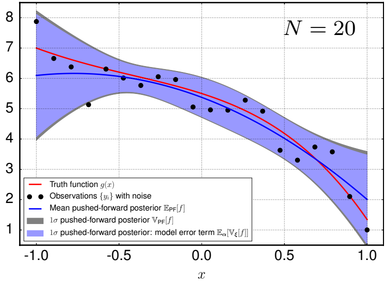


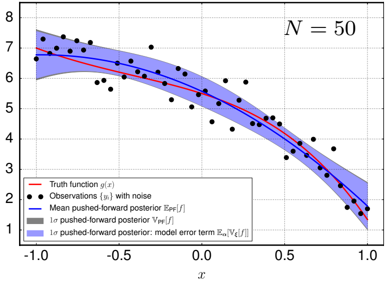


- With additional data, predictive uncertainty around the wrong model is indefinitely reducible
- Predictive uncertainty not indicative of discrepancy from truth

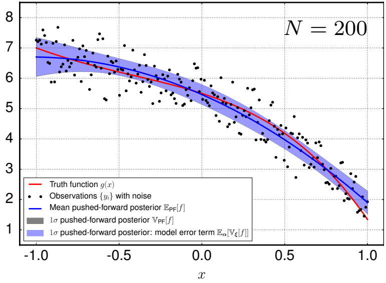


Quadratic-fit – ModErr – MargGauss

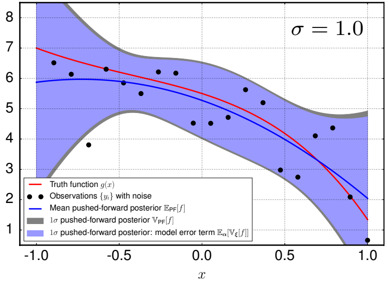


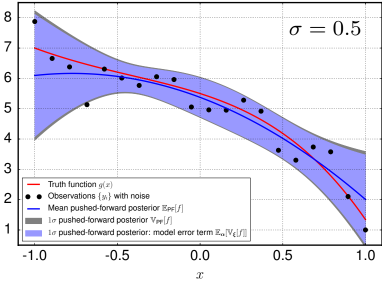


- With additional data, predictive uncertainty due to data noise is reducible
- Predictive uncertainty due to model error is not reducible

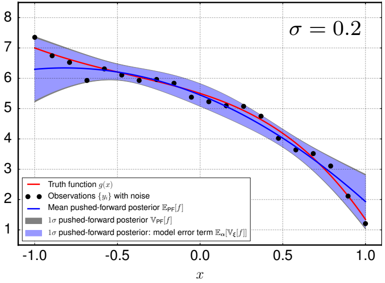


Quadratic-fit – ModErr – MargGauss

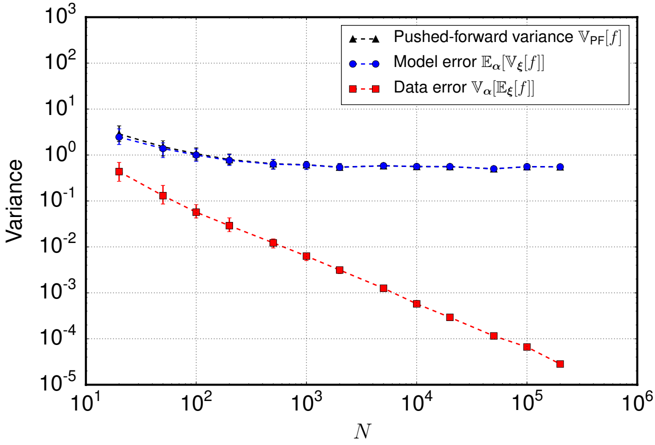




- Predictive uncertainty composed of both model-error and data-noise components
- The data-noise component is reducible with lower-noise in the data

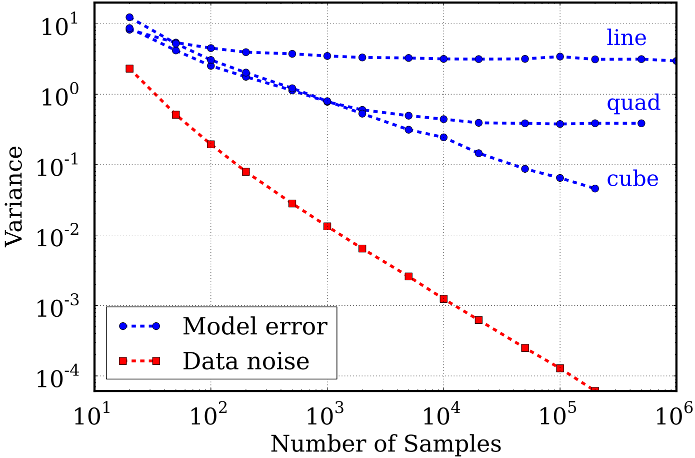


Quadratic-fit – ModErr – MargGauss



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



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
- Uncertainty due to data-noise:
  - Manifested in $\mathbb{V}_\alpha[\mathbb{E}_\xi[f]]$ – Reducible with more/cleaner data
- Uncertainty due to model-error:
  - Manifested in $\mathbb{E}_\alpha[\mathbb{V}_\xi[f]]$ – Not reducible