Uncertainty Quantification in Computational Models

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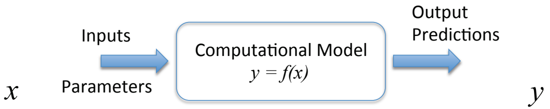
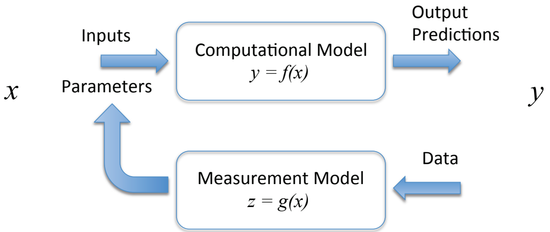
Uncertainty Quantification and Computational Science



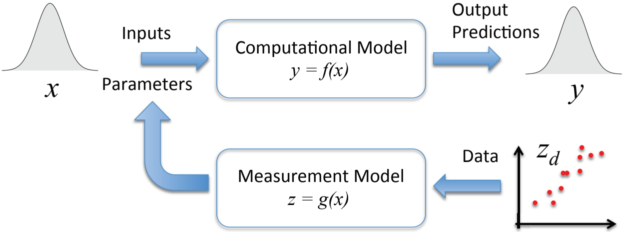
Forward problem

Uncertainty Quantification and Computational Science



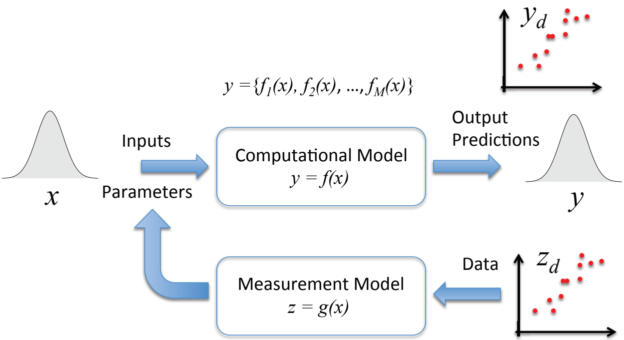
Inverse & Forward problems

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Model validation & comparison, Hypothesis testing

Outline

Forward propagation of parametric uncertainty

Forward model: $y = f(x)$

- Local sensitivity analysis (SA) and error propagation

$$\Delta y = \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} \Delta x$$

  This is ok for:

  - small uncertainty
  - low degree of non-linearity in $f(x)$

- Non-probabilistic methods
  - Fuzzy logic
  - Evidence theory – Dempster-Shafer theory
  - Interval math

- Probabilistic methods – this is our focus

Probabilistic Forward UQ – $y = f(x)$

Represent uncertain quantities using probability theory

- Random sampling, MC, QMC
  - Generate random samples $\{x^i\}_{i=1}^N$ from the PDF of x, $p(x)$
  - Bin the corresponding $\{y^i\}$ to construct $p(y)$
  - Not feasible for computationally expensive $f(x)$
    - slow convergence of MC/QMC methods
      $\Rightarrow$ very large N required for reliable estimates
- Build a cheap surrogate for $f(x)$, then use MC
  - Collocation – interpolants
  - Regression – fitting
- Galerkin methods
  - Polynomial Chaos (PC)
  - Intrusive and non-intrusive PC methods

Probabilistic Forward UQ & Polynomial Chaos Representation of Random Variables

With $y = f(x)$, x a random variable, estimate the RV y

- Can describe a RV in terms of its
  - density, moments, characteristic function, or
  - as a function on a probability space
- Constraining the analysis to RVs with finite variance
  $\Rightarrow$ Represent RV as a spectral expansion in terms of orthogonal functions of standard RVs
    - Polynomial Chaos Expansion
- Enables the use of available functional analysis methods for forward UQ

Polynomial Chaos Expansion (PCE)

- Model uncertain quantities as random variables (RVs)
- 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:

$$u(\boldsymbol{x}, t, \omega) = f(\boldsymbol{x}, t, \boldsymbol{\xi}) \simeq \sum_{k=0}^{P} u_k(\boldsymbol{x}, t) \Psi_k(\boldsymbol{\xi}(\omega))$$

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

Orthogonality

By construction, the functions $\Psi_k()$ are orthogonal with respect to the density of ξ

$$u_k(\boldsymbol{x}, t) \quad = \quad \frac{\langle u \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{\langle \Psi_k^2 \rangle} \int u(\boldsymbol{x}, t; \lambda(\boldsymbol{\xi})) \Psi_k(\boldsymbol{\xi}) \; p_{\boldsymbol{\xi}}(\boldsymbol{\xi}) \; d\boldsymbol{\xi}$$

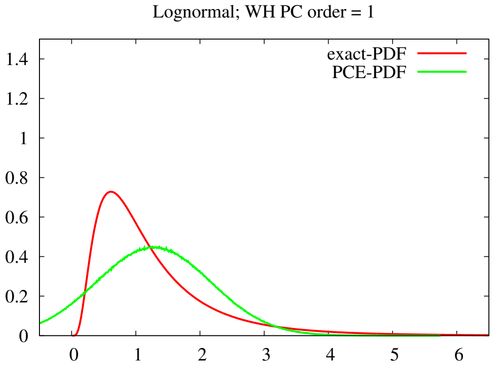
Examples:

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

PC Illustration: WH PCE for a Lognormal RV

- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 1

$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1 \xi
\end{aligned}
$$

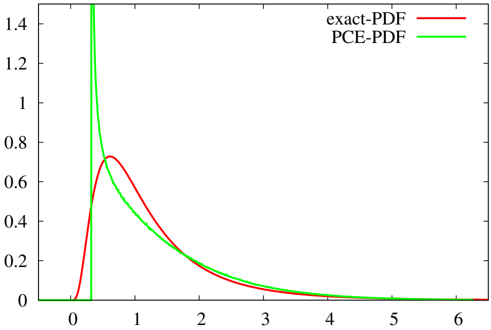


PC Illustration: WH PCE for a Lognormal RV

- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 2

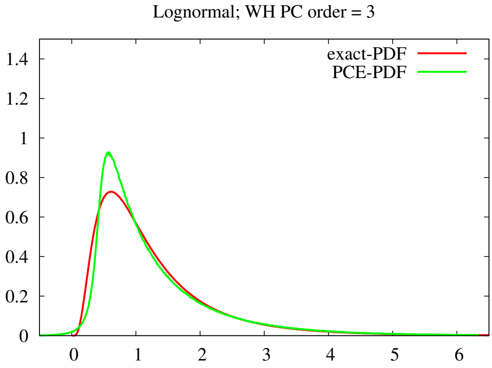
$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1)
\end{aligned}
$$

Lognormal; WH PC order = 2



PC Illustration: WH PCE for a Lognormal RV

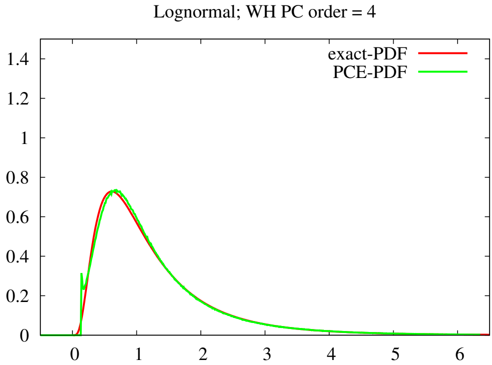
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 3



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi)
\end{aligned}
$$

PC Illustration: WH PCE for a Lognormal RV

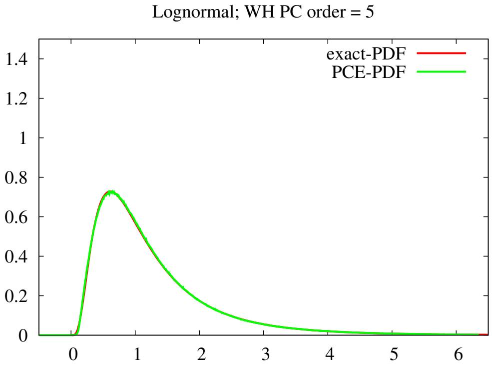
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 4



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3)
\end{aligned}
$$

PC Illustration: WH PCE for a Lognormal RV

- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 5



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3) \\
&\quad + u_5(\xi^5 - 10\xi^3 + 15\xi)
\end{aligned}
$$

Random Fields

- A random variable is a function on an event space Ω
  - No dependence on other coordinates –*e.g.* space or time
- A random field is a function on a product space $\Omega \times D$
  - *e.g.* sea surface temperature $T_{\mathrm{ss}}(z, \omega)$, $z \equiv (\boldsymbol{x}, t)$
- It is a more complex object than a random variable
  - A combination of an infinite number of random variables
- In many physical systems, uncertain field quantities, described by random fields:
  - are smooth, *i.e.*
  - they have an underlying *low dimensional structure*

  due to large correlation length-scales

Random Fields – KLE

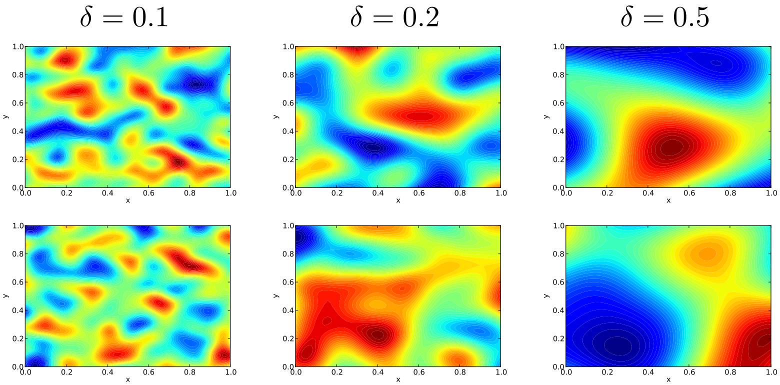
- Smooth random fields can be represented with a small no. of stochastic degrees of freedom
- A random field $M(x, \omega)$ with
  - a mean function: $\mu(x)$
  - a continuous covariance function: $C(x_1, x_2) = \langle [M(x_1, \omega) - \mu(x_1)][M(x_2, \omega) - \mu(x_2)] \rangle$

  can be represented with the Karhunen-Loeve Expansion (KLE)

$$M(x, \omega) = \mu(x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \eta_i(\omega) \phi_i(x)$$

  where
  - λ_i and $\phi_i(x)$ are the eigenvalues and eigenfunctions of the covariance function $C(\cdot, \cdot)$
  - η_i are uncorrelated zero-mean unit-variance RVs
- KLE $\Rightarrow$ representation of random fields using PC

RF Illustration: KL of 2D Gaussian Process

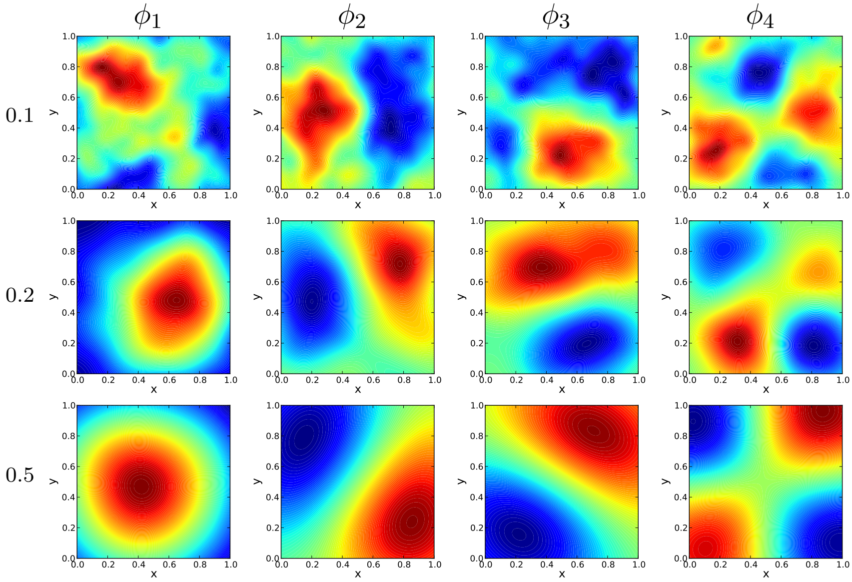


- 2D Gaussian Process with covariance:

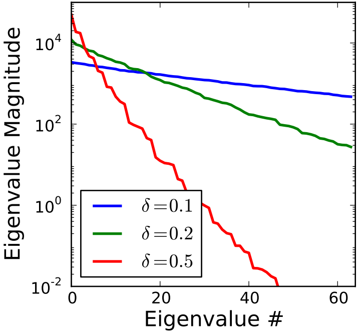
$$C(x_1, x_2) = \text{exp}(-||x_1 - x_2||^2/\delta^2)$$

- Realizations smoother as covariance length δ increases

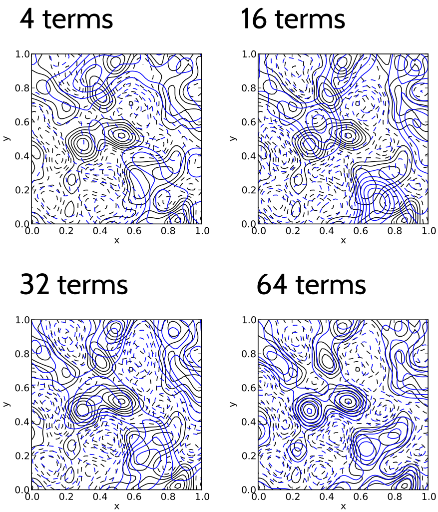
RF Illustration: 2D KL - Modes for $\delta = 0.1 - 0.5$



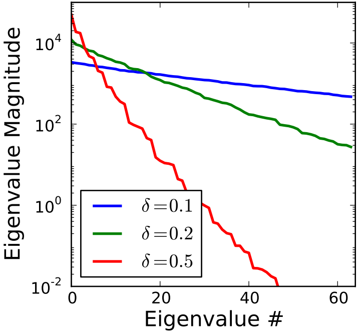
RF Illustration: 2D KL - eigenvalue spectrum



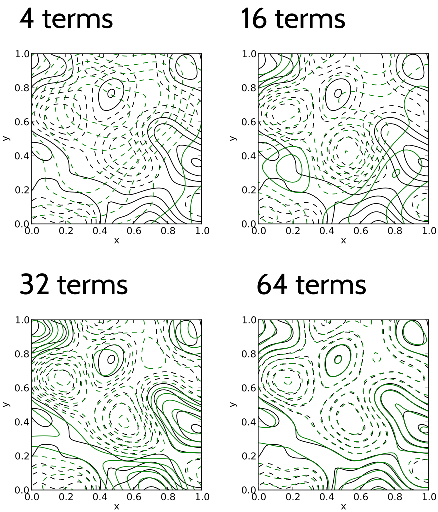
$\delta = 0.1$



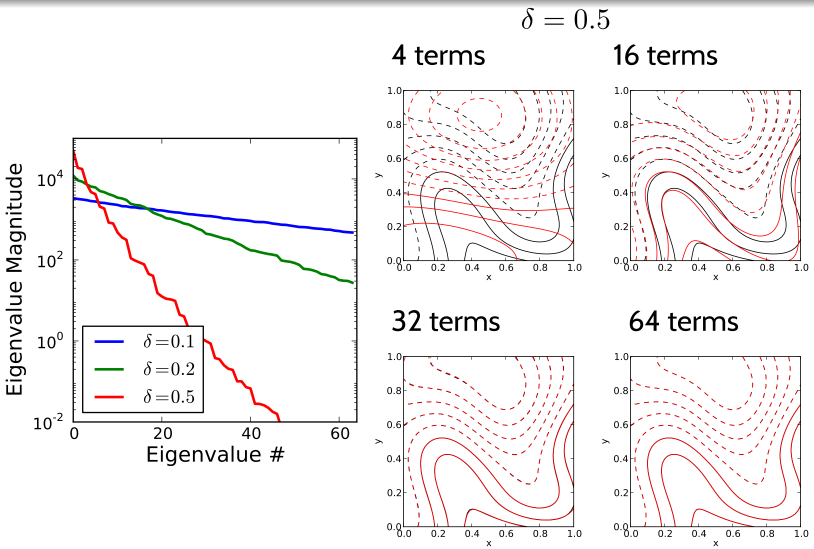
RF Illustration: 2D KL - eigenvalue spectrum



$\delta = 0.2$



RF Illustration: 2D KL - eigenvalue spectrum



Essential Use of PC in UQ

Strategy:

- Represent model parameters/solution as random variables
- Construct PCEs for uncertain parameters
- Evaluate PCEs for model outputs

Advantages:

- Computational efficiency
- Utility
  - Moments: $\mathsf{E}(u) = u_0$, $\mathsf{var}(u) = \sum_{k=1}^{P} u_k^2 \langle \Psi_k^2 \rangle$, ...
  - Global Sensitivities – fractional variances, Sobol' indices
  - Surrogate for forward model

Requirement:

- RVs in L^2, *i.e.* with finite variance, on $(\Omega, \mathfrak{S}(\boldsymbol{\xi}), P)$

Intrusive PC UQ: A direct *non-sampling* method

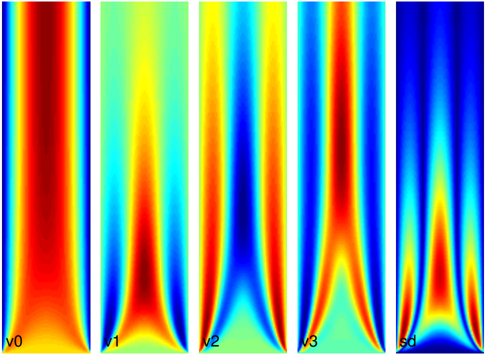
- Given model equations: $\boxed{\mathcal{M}(u(\boldsymbol{x},t);\lambda)=0}$
- Express uncertain parameters/variables using PCEs

$$u=\sum_{k=0}^{P} u_k\Psi_k; \quad \lambda=\sum_{k=0}^{P} \lambda_k\Psi_k$$

- Substitute in model equations; apply Galerkin projection
- New set of equations: $\boxed{\mathcal{G}(U(\boldsymbol{x},t),\Lambda)=0}$
  - with $U=[u_0,\ldots,u_P]^T$, $\Lambda=[\lambda_0,\ldots,\lambda_P]^T$
- Solving this <u>deterministic</u> system <u>once</u> provides the full specification of uncertain model ouputs

Laminar 2D Channel Flow with Uncertain Viscosity

- Incompressible flow
- Viscosity PCE
  - $\nu = \nu_0 + \nu_1 \xi$
- Streamwise velocity
  - $\mathsf{v} = \sum_{i=0}^{P} \mathsf{v}_i \Psi_i$
  - v_0: mean
  - v_i: i-th order mode
  - $\sigma^2 = \sum_{i=1}^{P} \mathsf{v}_i^2 \langle \Psi_i^2 \rangle$



v_0 v_1 v_2 v_3 σ

(Le Maître *et al.*, J. Comput. Phys., 2001)

Intrusive PC UQ Pros/Cons

Cons:

- Reformulation of governing equations
- New discretizations
- New numerical solution method
  - Consistency, Convergence, Stability
  - Global vs. multi-element local PC constructions
- New solvers and model codes
  - Opportunities for automated code transformation
- New preconditioners

Pros:

- Tailored solvers can deliver superior performance

Non-intrusive PC UQ

- *Sampling*-based
- Relies on black-box utilization of the computational model
- Evaluate projection integrals *numerically*
- For any quantity of interest $\phi(\boldsymbol{x},t;\lambda) = \sum_{k=0}^{P} \phi_k(\boldsymbol{x},t)\Psi_k(\boldsymbol{\xi})$

$$\phi_k(\boldsymbol{x},t) = \frac{1}{\langle \Psi_k^2 \rangle} \int \phi(\boldsymbol{x},t;\lambda(\boldsymbol{\xi}))\, \Psi_k(\boldsymbol{\xi}) p_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad k = 0,\ldots,P$$

- Integrals can be evaluated using
  - A variety of (Quasi) Monte Carlo methods
    - Slow convergence; $\sim$ indep. of dimensionality
  - Quadrature/Sparse-Quadrature methods
    - Fast convergence; depends on dimensionality

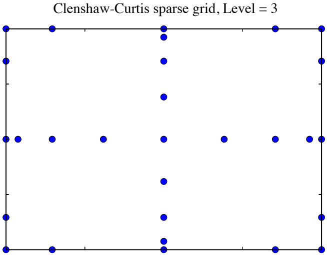
PC and High-Dimensionality

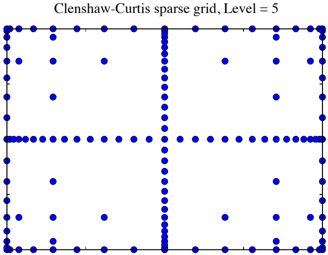
Dimensionality n of the PC basis: $\boldsymbol{\xi} = \{\xi_1, \ldots, \xi_n\}$

- $n \approx$ number of uncertain parameters
- $P + 1 = (n + p)!/n!p!$ grows fast with n

Impacts:

- Size of intrusive PC system
- Hi-D projection integrals $\Rightarrow$ large # non-intrusive samples
  - Sparse quadrature methods

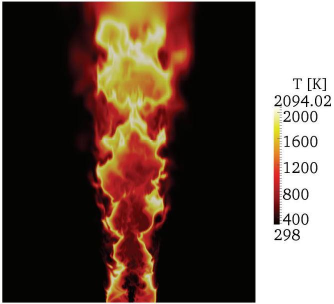


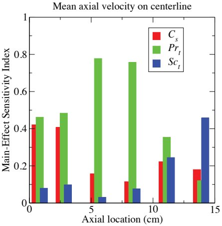


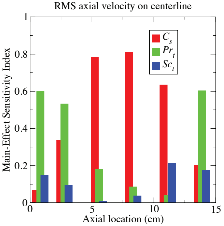
UQ in LES computations: turbulent bluff-body flame

with M. Khalil, G. Lacaze, & J. Oefelein, Sandia Nat. Labs

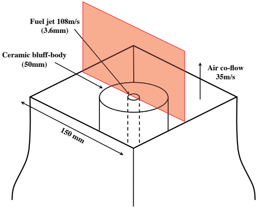
- CH_4-H_2 jet, air coflow, 3D flow
- Re=9500, LES subgrid modeling
- 12×10^6 mesh cells, 1024 cores
- 3 days run time, 2×10^5 time steps
- 3 uncertain parameters (C_s, Pr_t, Sc_t)
- 2^{nd}-order PC, 25 sparse-quad. pts







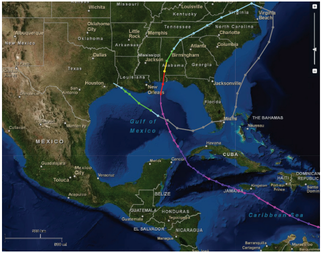
Main-Effect Sensitivity Indices

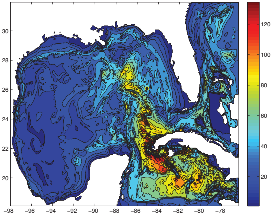


J. Oefelein & G. Lacaze, SNL

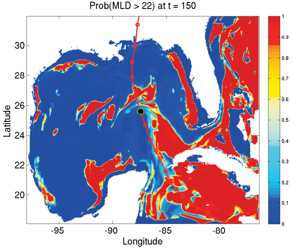
UQ in Ocean Modeling – Gulf of Mexico

A. Alexanderian, J. Winokur, I. Sraj, O.M. Knio, Duke Univ.
A. Srinivasan, M. Iskandarani, Univ. Miami; W.C. Thacker, NOAA





- Hurricane Ivan, Sep. 2004
- HYCOM ocean model (hycom.org)
- Predicted Mixed Layer Depth (MLD)
- Four uncertain parameters, *i.i.d.* U
  - subgrid mixing & wind drag params
- 385 sparse quadrature samples



(Alexanderian *et al.*, Winokur *et. al.*, *Comput. Geosci.*, 2012, 2013)

Inverse UQ – Estimation of Uncertain Parameters

Forward UQ requires specification of uncertain inputs

Probabilistic setting

- Require joint PDF on input space
- Statistical inference – an inverse problem

Bayesian setting

- Given Data: PDF on uncertain inputs can be estimated using Bayes formula
  - Bayesian Inference
- Given Constraints: PDF on uncertain inputs can be estimated using the Maximum Entropy principle
  - MaxEnt Methods

Bayes formula for Parameter Inference

- Data Model (fit model + noise model): $y = f(\lambda) * g(\epsilon)$
- Bayes Formula:

$$p(\lambda, y) = p(\lambda|y)p(y) = p(y|\lambda)p(\lambda)$$

$$\underbrace{p(\lambda|y)}_{\text{Posterior}} = \frac{\overbrace{p(y|\lambda)}^{\text{Likelihood}}\;\overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- Prior: knowledge of λ prior to data
- Likelihood: forward model and measurement noise
- Posterior: combines information from prior and data
- Evidence: normalizing constant for present context

The Prior

- Prior $p(\lambda)$ comes from
  - Physical constraints
  - Prior data
  - Prior knowledge
- The prior can be **uninformative**
- It can be chosen to impose **regularization**
- Unknown aspects of the prior can be added to the rest of the parameters as hyperparameters
- The choice of prior can be crucial when there is little information in the data relative to the number of degrees of freedom in the inference problem
- When there is sufficient information in the data, the data can overrule the prior

Construction of the Likelihood $p(y|\lambda)$

- Where does probability enter the mapping $\lambda \to y$ in $p(y|\lambda)$?
- Through a presumed error model:
- Example:
  - Model:

$$y_m = g(\lambda)$$

  - Data: y
  - Error between data and model prediction: ϵ

$$y = g(\lambda) + \epsilon$$

- Model this error as a random variable
- Example
  - Error is due to instrument measurement noise
  - Instrument has Gaussian errors, with no bias

$$\epsilon \sim N(0, \sigma^2)$$

Construction of the Likelihood $p(y|\lambda)$ - cont'd

For any given λ, this implies

$$y|\lambda, \sigma \sim N(g(\lambda), \sigma^2)$$

or

$$p(y|\lambda, \sigma) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{(y - g(\lambda))^2}{2\sigma^2}\right)$$

Given N measurements $(y_1, \ldots, y_N)$, and presuming independent identically distributed (*iid*) noise

$$\begin{aligned} y_i &= g(\lambda) + \epsilon_i \\ \epsilon_i &\sim N(0, \sigma^2) \\ L(\lambda) = p(y_1, \ldots, y_N|\lambda, \sigma) &= \prod_{i=1}^{N} p(y_i|\lambda, \sigma) \end{aligned}$$

Likelihood Modeling

- This is frequently the *core* modeling challenge
  - Error model: a statistical model for the discrepancy between the forward model and the data
  - composition of the error model with the forward model
- Error model composed of discrepancy between
  - data and the truth – (data error)
  - model prediction and the truth – (model error)
- Mean bias and correlated/uncorrelated noise structure
- Hierarchical Bayes modeling, and dependence trees

$$p(\phi, \theta | D) = p(\phi | \theta, D) p(\theta | D)$$

- Choice of observable – constraint on Quantity of Interest?

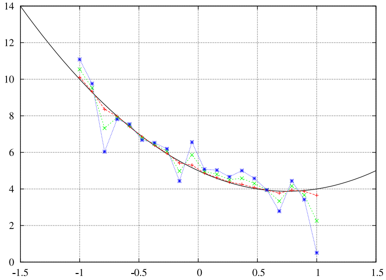
Exploring the Posterior

- Given any sample λ, the un-normalized posterior probability can be easily computed

$$p(\lambda|y) \propto p(y|\lambda)p(\lambda)$$

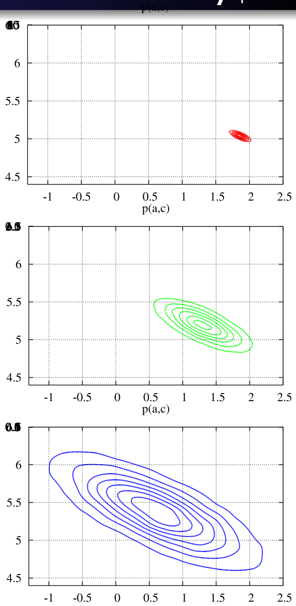
- Explore posterior w/ Markov Chain Monte Carlo (MCMC)
  - Metropolis-Hastings algorithm:
    - Random walk with proposal PDF & rejection rules
  - Computationally intensive, $\mathcal{O}(10^5)$ samples
  - Each sample: evaluation of the forward model
    - Surrogate models
- Evaluate moments/marginals from the MCMC statistics

Bayesian inference illustration: noise$\uparrow \Rightarrow$ uncertainty$\uparrow$



- data: $y = 2x^2 - 3x + 5 + \epsilon$
- $\epsilon \sim \mathcal{N}(0, \sigma^2)$, $\sigma = \{0.1, 0.5, 1.0\}$
- Fit model $y = ax^2 + bx + c$

Marginal posterior density $p(a, c)$:



Bayesian inference – High Dimensionality Challenge

- Judgement on local/global posterior peaks is difficult
  - Multiple chains; Tempering
- Choosing a good starting point is very important
  - An initial optimization strategy is useful, albeit not trivial
- Choosing good MCMC proposals, and attaining good mixing
  - Likelihood-informed
    - Markov jump in those dimensions informed by data
    - Sample from prior in complement of dimensions
    - Adaptive proposal learning from MCMC samples
    - Log-Posterior Hessian $\Rightarrow$ local Gaussian approx.
    - Adaptive, Geometric, Langevin MCMC
  - Dimension independent
    - Proposal design: good MCMC performance in hiD
  - Literature: A. Stuart, M. Girolami, K. Law, T. Cui, Y. Marzouk

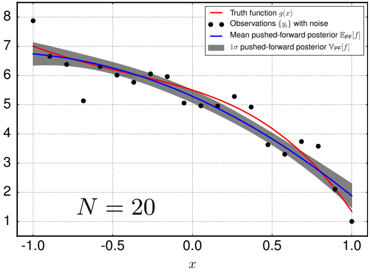
(Law 2014; Cui *et al.*, 2014,2015; Cotter *et al.*, 2013)

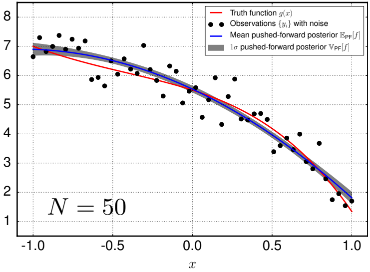
Bayesian inference – Model Error Challenge

- Quantifying model error, as distinct from data noise, is important for assessing confidence in model validity
- Conventional statistical methods for representation of model error have shortcomings when applied to physical models
- New methods are under-development for model error:
  - physical constraints are satisfied
  - feasible disambiguation of model-error/data-noise
  - calibrated model error terms adequately impact all model outputs of interest
  - uncertainties in predictions from calibrated model reflect the range of discrepancy from the truth
- Embed model error in submodel components where approximations exist

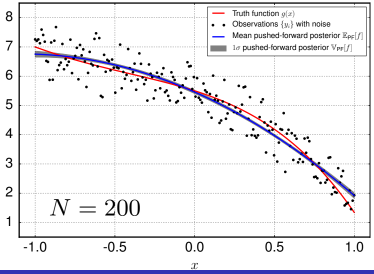
(K. Sargsyan *et al.*, 2015)

Quadratic-fit – Classical Bayesian likelihood

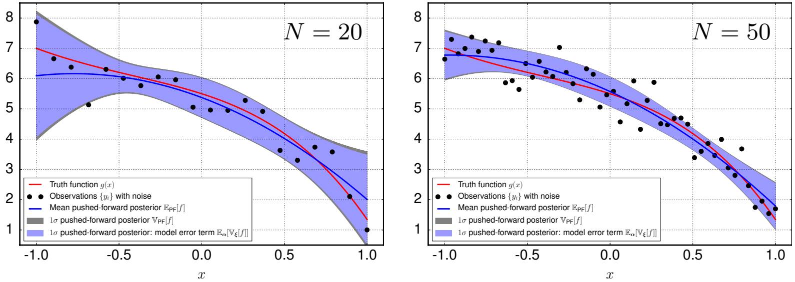




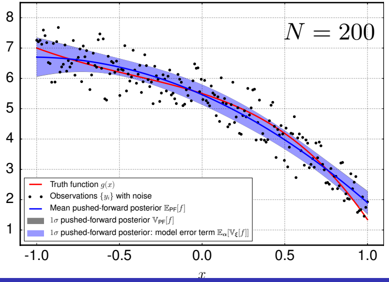
- With additional data, predictive uncertainty around the wrong model is indefinitely reducible
- Predictive uncertainty not indicative of discrepancy from truth



Quadratic-fit – ModErr – MargGauss



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



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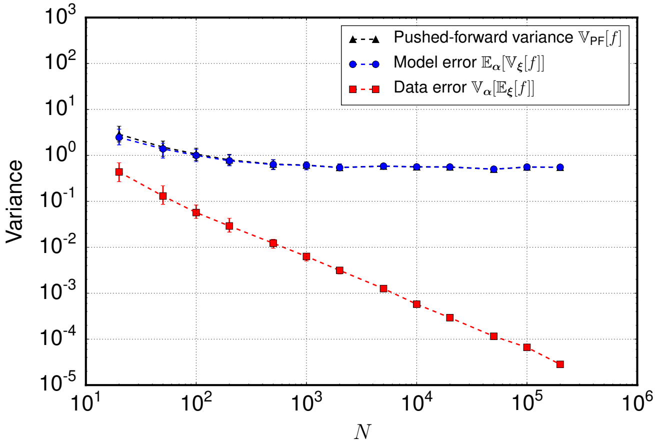


Calibrating a quadratic $f(x)$ w.r.t. $g(x) = 6 + x^2 + 0.5(x+1)^{3.5}$

Model Evidence and Complexity

Let $\mathcal{M} = \{M_1, M_2, \ldots\}$ be a set of models of interest

- Parameter estimation from data is conditioned on the model

$$p(\theta|D, M_k) = \frac{p(D|\theta, M_k)\pi(\theta|M_k)}{p(D|M_k)}$$

Evidence (marginal likelihood) for M_k:

$$p(D|M_k) = \int p(D|\theta, M_k)\pi(\theta|M_k)\mathrm{d}\theta$$

Model evidence is useful for model selection

- Choose model with maximum evidence
- Compromise between fitting data and model complexity
  - Optimal complexity – Occam's razor principle
  - Avoid overfitting

Too much model complexity leads to overfitting

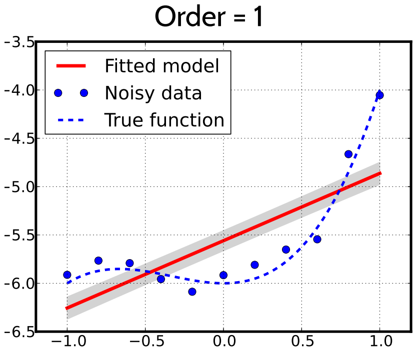
Data model: $i = 1, \ldots, N$

$$\begin{aligned} y_i &= x_i^3 + x_i^2 - 6 + \epsilon_i \\ \epsilon_i &\sim N(0, s) \end{aligned}$$

Bayesian regression with Legendre PCE fit models, order 1-10

$$y_m = \sum_{k=0}^{P} c_k \psi_k(x)$$

Uniform priors $\pi(c_k)$, $k = 0, \ldots, P$



Fitted model pushed-forward posterior versus the data

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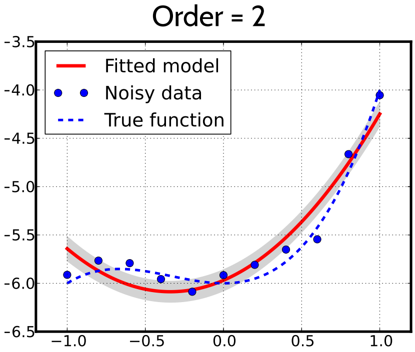

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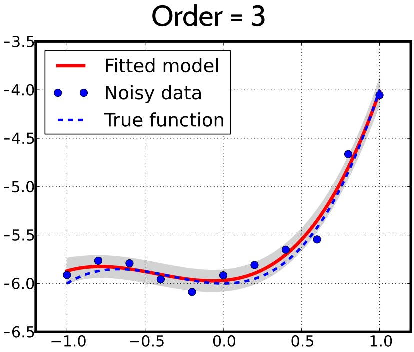

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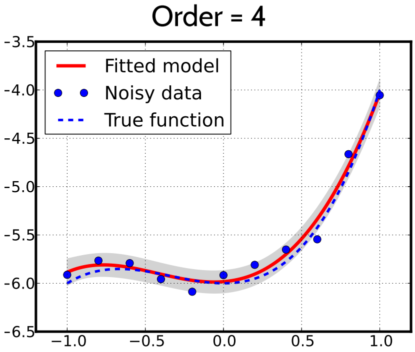

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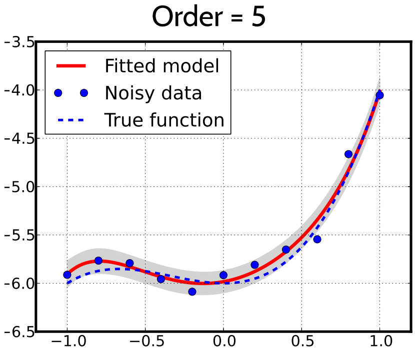

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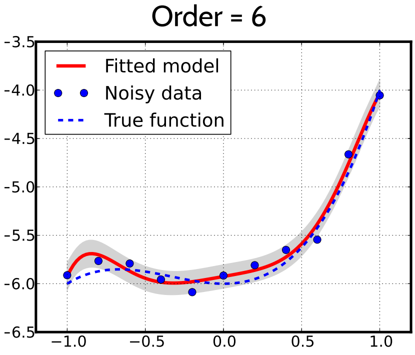

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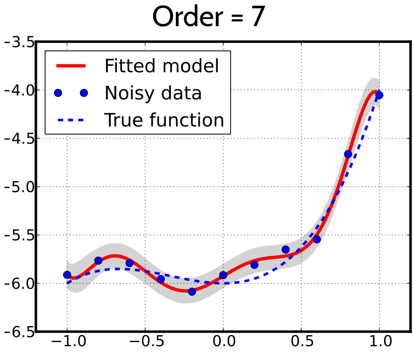

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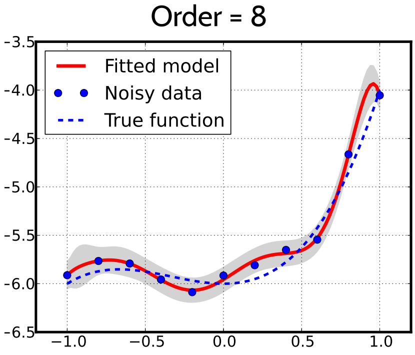

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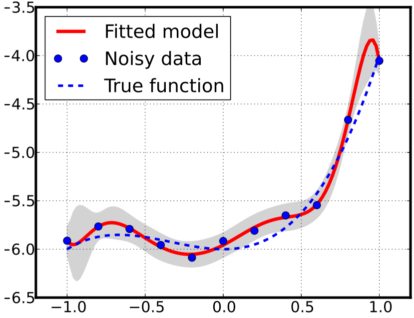
Order = 9



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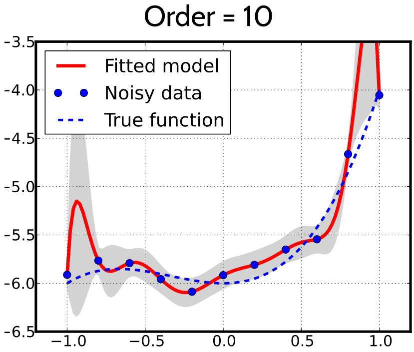
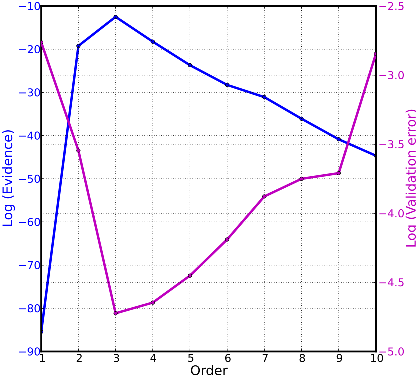


Fitted model pushed-forward posterior versus the data

Evidence and Cross-Validation Error

- Model evidence peaks at the true polynomial order of 3
- Cross validation error is equally minimal at order 3
- Models with optimal complexity are robust to cross validation



Cross validation error and model evidence versus order

Closure

- Probabilistic UQ framework
  - Polynomial Chaos representation of random variables
- Forward UQ
  - Intrusive and non-intrusive forward PC UQ methods
- Inverse UQ
  - Parameter estimation via Bayesian inference
  - Model error
  - Model complexity
- Challenges
  - High dimensionality
  - Intrusive Galerkin stability
  - Nonlinearity
  - Time dynamics
  - Model error