Probabilistic Methods for Uncertainty Quantification in Computational Models

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Livermore, CA

Schlumberger,
Inversion, Optimization & Uncertainty
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Outline

Background

- Ph.D. from U. of Michigan, Applied Math,, 2007
- 2007-present: working in UQ at Sandia National Labs

- US Department of Energy, Office of Science, Advanced Scientific Computing Research (ASCR)
- QUEST Institute (Quantification of Uncertainty in Extreme Scale CompuTations)
    - PI: Habib Najm
    - www.quest-scidac.org
    - Advanced UQ methods development
    - Reach out to application community
- SNL-CA: 5-10 staff members, $\sim$ 5 postdocs
    - Main research code: UQTk (www.sandia.gov/UQToolkit)
        - Lightweight C++/Python codebase
        - UQTk v3.0 to be posted soon

UQ Software Packages under QUEST

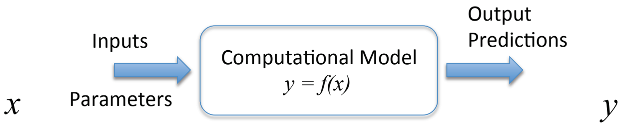
- The SciDAC Institute on Quantification of Uncertainty in Extreme Scale Computations (QUEST) is developing and maintaining a number of packages
  - `http://www.quest-scidac.org/`
  - DAKOTA: `http://dakota.sandia.gov/`
  - UQTk: UQ Toolkit `http://www.sandia.gov/UQToolkit/`
  - GPMSA: Gaussian Process Modeling and Sensitivity Analysis
  - QUESO: Bayesian inference `https://github.com/libqueso/queso/releases`
  - MUQ: MIT Uncertainty Quantification library `https://bitbucket.org/mituq/muq`
- Many packages are becoming available outside QUEST (UQLab, OpenTurns, SmartUQ, ChaosPy,...)

Uncertainty Quantification Toolkit (UQTk)

- A library of C++ and Python functions for propagation of uncertainty through computational models
- Mainly relies on Polynomial Chaos (PC) expansions for representing random variables and stochastic processes
- Target usage:
  - Rapid prototyping
  - Algorithmic research
  - Tutorials / educational
- Version 2.1 released under the GNU Lesser General Public License
  - C++ Tools for intrusive and non-intrusive UQ
  - Polynomial Chaos
  - Bayesian inference tools (various MCMC types)
  - Regression (polynomial, RBF, GP) tools
  - (Sparse) quadrature integration
  - Rosenblatt transformation
  - Python postprocessing and analysis tools
- Version 3.0 to be released very soon
- Available at `http://www.sandia.gov/UQToolkit`

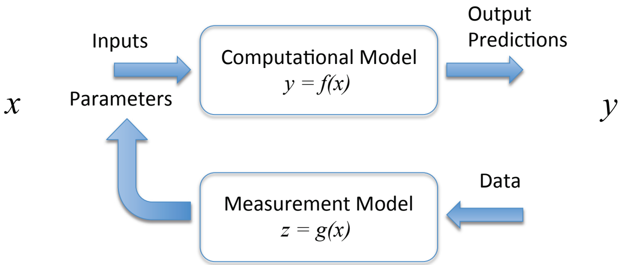
UQTk

Uncertainty Quantification and Computational Science



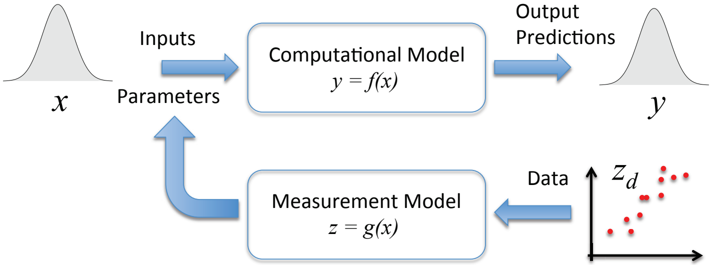
Forward problem

Uncertainty Quantification and Computational Science



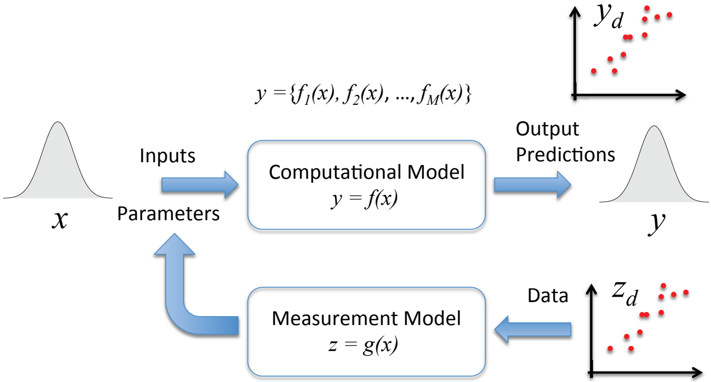
Inverse & Forward problems

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Uncertainty Quantification and Computational Science



Inverse & Forward UQ

Model validation & comparison, Hypothesis testing

The Case for Uncertainty Quantification

UQ needed for...

- Model predictions
- Model validation and comparison
- Confidence assessment
- Reliability analysis
- Dimensionality reduction
- Optimal design
- Decision support
- (Noisy) data assimilation

Uncertainty Sources

- Model parameters
- Initial/boundary conditions
- Model geometry/structure
- Lack of knowledge
- Data noise
- Intrinsic stochasticity
- Numerical errors, too

Outline

Polynomial Chaos – functional representation for RVs

$$U \simeq \sum_{k=0}^{p} u_k \psi_k(\xi)$$

- First introduced by Wiener, 1938
- Revitalized by Ghanem and Spanos, 1991
- Convergent series if U has finite variance
- Selection of order p is a modeling choice
- Describes a r.v. U with a vector of *PC modes* $(u_0, u_1, \dots, u_p)$

- Standard r.v. ξ, standard orthogonal polynomials $\psi_k(\xi)$, *i.e.*

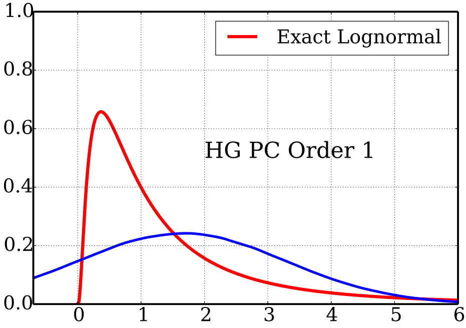
$$\int \psi_i(\xi)\psi_j(\xi)\pi_\xi(\xi)d\xi = \delta_{ij}||\psi_i||^2$$

PC Type	Domain	Density $\pi_\xi(\xi)$	Polynomial	Free parameters
Gauss-Hermite	$(-\infty, +\infty)$	$\frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}}$	Hermite	none
Legendre-Uniform	$[-1, 1]$	$\frac{1}{2}$	Legendre	none
Gamma-Laguerre	$[0, +\infty)$	$\frac{\xi^\alpha e^{-\xi}}{\Gamma(\alpha+1)}$	Laguerre	$\alpha > -1$
Beta-Jacobi	$[-1, 1]$	$\frac{(1+\xi)^\alpha(1-\xi)^\beta}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}$	Jacobi	$\alpha > -1, \beta > -1$

[Wiener, 1938; Ghanem & Spanos, 1991; Xiu & Karniadakis, 2002; Le Maître & Knio, 2010]

Construction of 1D PC $U \simeq \sum_{k=0}^{p} u_k \psi_k(\xi)$

- Orthogonal projection: $u_k = \frac{1}{||\psi_k||^2}\langle U\psi_k\rangle$
- Need to compute integral $\langle U\psi_k\rangle = \int U(?)\psi_k(\xi)\pi_\xi(\xi)d\xi$
- Need a map $U \leftrightarrow \xi$
- If lucky, there is an explicit formula, e.g. lognormal $U = e^{\xi}$



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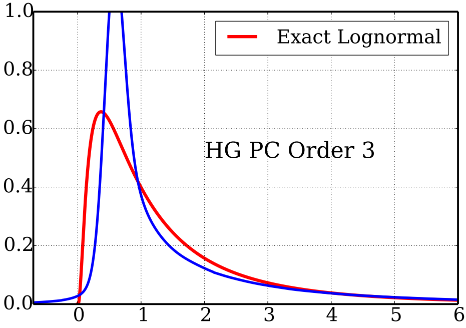

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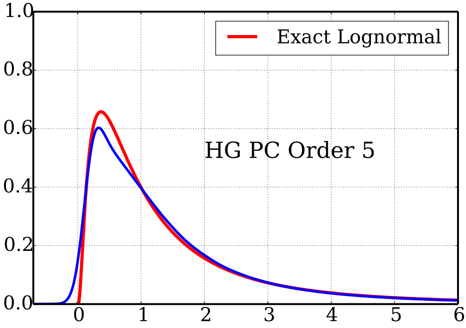

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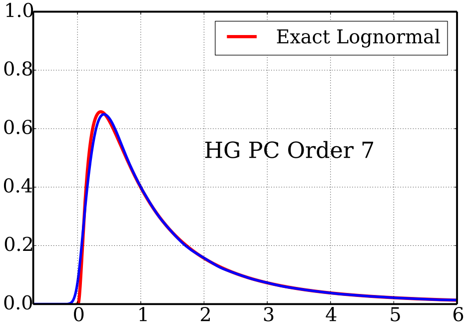

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- CDF transform helps:
  - $U = F_U^{-1}(\frac{\xi+1}{2})$ if ξ is Uniform, Legendre-Uniform PC
  - $U = F_U^{-1}(\Phi(\xi))$ if ξ is Normal, Gauss-Hermite PC

where $F_U(\cdot)$ is the Cumulative Distribution Function (CDF) of U.

[and $\Phi(\cdot)$ is CDF for standard normal]

Multivariate Polynomial Chaos

$$
\begin{cases}
U_1 = \sum_{k=0}^{K_1} u_{1k} \Psi_k(\xi_1, \dots, \xi_n) \\
U_2 = \sum_{k=0}^{K_2} u_{2k} \Psi_k(\xi_1, \dots, \xi_n) \\
\vdots \qquad\qquad \vdots \\
U_d = \sum_{k=0}^{K_d} u_{dk} \Psi_k(\xi_1, \dots, \xi_n)
\end{cases}
$$

- Multivariate polynomial $\Psi_k(\boldsymbol{\xi}) = \psi_{\alpha_1}(\xi_1) \cdots \psi_{\alpha_n}(\xi_n)$
- Usually $d = n$
- Construction non-trivial: e.g., capture
  - the PDF of U
  - select moments of U
  - some QoI $h(U)$
- Multivariate normal is a special case
- Multiindex $(\alpha_1, \dots, \alpha_n)$ selection, Truncation; see later
- Rosenblatt map (multivariate CDF transform)

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Fun example: $X = \xi_1^2 + \xi_2^2$ is exponential r.v. if ξ's are i.i.d. gaussians. However, no finite order 1D PC exists.

Essential Use of PC in UQ

$U \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$

Strategy:

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

Advantages:

- Computational efficiency
- Utility
  - Moments: $\mathbb{E}[u] = u_0, \ \mathbb{V}[u] = \sum_{k=1}^{K} u_k^2 ||\Psi_k||^2, \ \ldots$
  - Global Sensitivities – fractional variances, Sobol' indices
  - Uncertainty propagation
  - Surrogate for forward model

Requirements:

- Finite variances (not a handicap in practice)
- Smooth forward functions

PC features: moment extraction

$$U \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$$

- Expectation: $\langle u \rangle = u_0$
- Variance σ^2

$$\begin{aligned}
\sigma^2 &= \left\langle (u - \langle u \rangle)^2 \right\rangle = \left\langle (\sum_{k=1}^{K} u_k \Psi_k(\boldsymbol{\xi}))^2 \right\rangle \\
&= \left\langle \sum_{k=1}^{K} \sum_{j=1}^{K} u_j u_k \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \right\rangle \\
&= \sum_{k=1}^{K} \sum_{j=1}^{K} u_j u_k \left\langle \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \right\rangle = \sum_{k=1}^{K} u_k^2 ||\Psi_k||^2
\end{aligned}$$

PC features: Global Sensitivity Analysis $U(\boldsymbol{\xi}) \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$

- Main effect sensitivity indices

$$S_i = \frac{Var[\mathbb{E}(U(\boldsymbol{\xi}|\xi_i)]}{Var[U(\boldsymbol{\xi})]} = \frac{\sum_{k\in\mathbb{I}_i} u_k^2 ||\Psi_k||^2}{\sum_{k>0} u_k^2 ||\Psi_k||^2}$$

  - $\mathbb{I}_i$ is the set of bases with only ξ_i involved
  - S_i is the uncertainty contribution that is due to i-th parameter only

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- Total effect sensitivity indices

$$T_i = 1 - \frac{Var[\mathbb{E}(U(\boldsymbol{\xi}|\xi_{-i})]}{Var[U(\boldsymbol{\xi})]} = \frac{\sum_{k\in\mathbb{I}_i^T} u_k^2 ||\Psi_k||^2}{\sum_{k>0} u_k^2 ||\Psi_k||^2}$$

$\mathbb{I}_i^T$ is the set of bases with ξ_i involved, including all its interactions.

PC features: Global Sensitivity Analysis $U(\boldsymbol{\xi}) \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$

- Main effect sensitivity indices

$$S_i = \frac{Var[\mathbb{E}(U(\boldsymbol{\xi}|\xi_i)]}{Var[U(\boldsymbol{\xi})]} = \frac{\sum_{k\in\mathbb{I}_i} u_k^2 ||\Psi_k||^2}{\sum_{k>0} u_k^2 ||\Psi_k||^2}$$

  - $\mathbb{I}_i$ is the set of bases with only ξ_i involved
  - S_i is the uncertainty contribution that is due to i-th parameter only

- Joint sensitivity indices

$$S_{ij} = \frac{Var[\mathbb{E}(U(\boldsymbol{\xi}|\xi_i,\xi_j)]}{Var[U(\boldsymbol{\xi})]} - S_i - S_j = \frac{\sum_{k\in\mathbb{I}_{ij}} u_k^2 ||\Psi_k||^2}{\sum_{k>0} u_k^2 ||\Psi_k||^2}$$

  - $\mathbb{I}_{ij}$ is the set of bases with only ξ_i and ξ_j involved
  - S_{ij} is the uncertainty contribution that is due to (i,j) parameter pair

PC features: uncertainty propagation

$$U \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$$

$$f(U) \simeq \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi})$$

- Basic task: given PC for inputs, find PC for outputs.
- Input-output map can also be defined implicitly, via governing equations $G(f, U) = 0$.
- Two approaches
  - Intrusive: project governing equations
    - Results in set of equations for the PC modes
    - Requires redesign of computer code
    - PCEs for all uncertain variables in system
  - Non-intrusive: project outputs of interest
    - Sampling to evaluate projection operator
    - Can use existing code as black box
    - Only computes PCEs for quantities of interest

Non-intrusive Spectral Projection (NISP) PC UQ

$$U \simeq \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$$

$$f(U) \simeq \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi})$$

- For any model output of interest $f(X)$:

$$f_k = \frac{\langle f \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{||\Psi_k||^2} \int f(X(\boldsymbol{\xi}))\, \Psi_k(\boldsymbol{\xi}) \pi_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

- Evaluate projection integral *numerically*
- Relies on black-box utilization of the computational model
- Integral 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 surrogate construction

- Build/presume PC for input parameter U

$$U(\boldsymbol{\xi}) = \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$$

with respect to multivariate standard polynomials.

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- E.g., uniform on an interval, or gaussian with known moments,

$$U = u_0 + u_1^T \boldsymbol{\xi}$$

PC surrogate construction

- Build/presume PC for input parameter U

$$U(\boldsymbol{\xi}) = \sum_{k=0}^{K} u_k \Psi_k(\boldsymbol{\xi})$$

with respect to multivariate standard polynomials.

- If input parameters are uniform $U_i \sim$ Uniform$[a_i, b_i]$, then

$$U_i = \frac{a_i + b_i}{2} + \frac{b_i - a_i}{2}\, \xi_i.$$

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with respect to multivariate standard polynomials.

- Input parameters are represented via their cumulative distribution function (CDF) $F(\cdot)$, such that, with $\xi_i \sim$ Uniform$[-1, 1]$

$$U_i = F_{U_i}^{-1}\left(\frac{\xi_i + 1}{2}\right), \qquad \text{for } i = 1, 2, \ldots, d.$$

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- Forward function $f(\cdot)$, output Z

$$Z = f(U(\boldsymbol{\xi})) \qquad Z = \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi}) \equiv f_s(\boldsymbol{\xi})$$

- Global sensitivity information for free
  - Sobol indices, variance-based decomposition.

Outline

Inverse UQ – Estimation of Uncertain Parameters

Probabilistic setting

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

Bayesian setting

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

Bayes formula for Parameter Inference

- Collected data: $\{(x_i, y_i)\}_{i=1}^N$
- Data model: $y_i = f(x_i; \lambda) + \epsilon_i$
- Bayes formula:

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

- 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/knowledge
- Types of *uninformative* priors
  - Improper prior
  - Objective prior
  - Maxent prior
  - Reference prior
  - Jeffreys prior

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

- 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 if data is not informative
- When there is sufficient information in the data, the data can overrule the prior

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

- Requires a presumed error model
- Data model: $y_i = f(x_i; \lambda) + \epsilon_i$

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

- Model this error as a random variable, e.g.
  - Error is due to instrument measurement noise
  - Instrument has Gaussian errors, with no bias
  - Measurements are independent

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

- For any given λ, this implies

$$y_i|\lambda, \sigma \sim N(f(x_i; \lambda), \sigma^2)$$

or

$$p(y|\lambda, \sigma) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{(y_i - f(x_i; \lambda))^2}{2\sigma^2}\right)$$

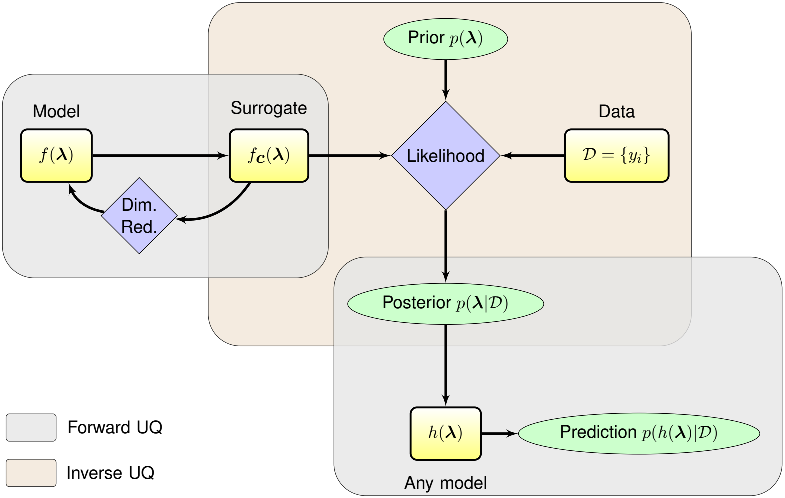
Exploring the Posterior

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

$$\underbrace{p(\lambda|y)}_{\text{Posterior}} \propto \underbrace{p(y|\lambda)}_{\text{Likelihood}} \underbrace{p(\lambda)}_{\text{Prior}}$$

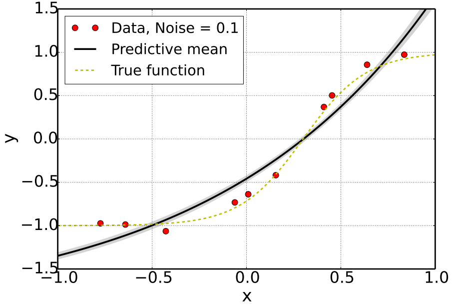
- Explore posterior w/ Markov Chain Monte Carlo (MCMC)
  - Metropolis-Hastings algorithm:
    - Random walk with proposal PDF & rejection rules
  - Computationally intensive, $\mathcal{O}(10^5)$ samples
  - Each sample: evaluation of the forward model
    - Surrogate models
- Evaluate moments/marginals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

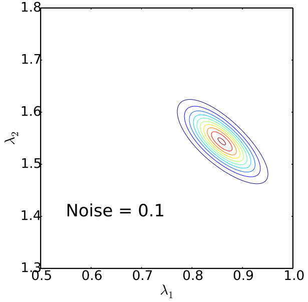
Forward and Inverse UQ in a workflow



Bayesian inference: Noise$\uparrow \Rightarrow$ Posterior uncertainty$\uparrow$

- True model $y = \tanh(3x - 0.9)$
- Increasing data noise level
- Calibrating $f(x; \lambda) = \lambda_1 e^{\lambda_0 x} - 2$
- Larger data noise $\Rightarrow$ larger posterior uncertainty





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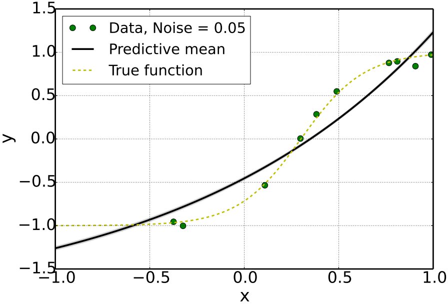

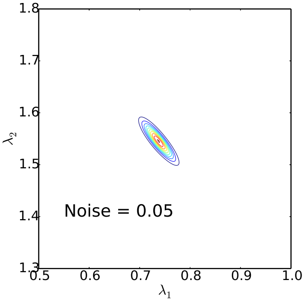

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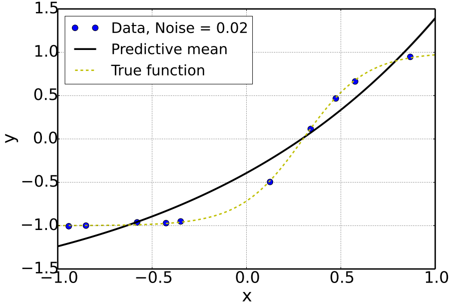

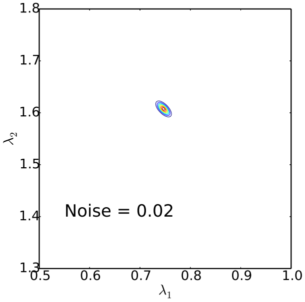

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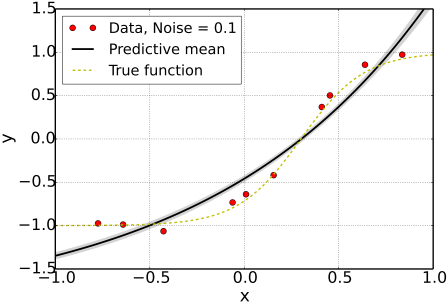
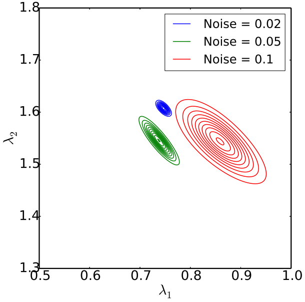
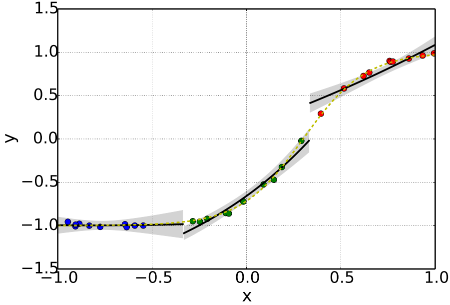
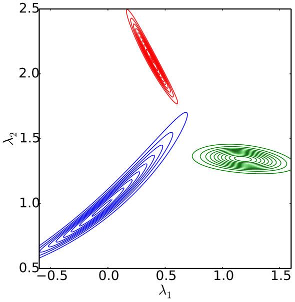




Bayesian inference: Data range $\Rightarrow$ Correlation

- True model $y = \tanh(3x - 0.9)$
- Collecting data at different locations
- Calibrating $f(x;\lambda) = \lambda_1 e^{\lambda_0 x} - 2$
- Correlation structure can change drastically





Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
- Intrinsic Stochasticity
- **Model Errors**
- Input Correlations
- Low-Probability (Tail) Events
- Time Dynamics

Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
  - Large number of input parameters
  - Dense spatial/temporal grid
  - PC truncation is a challenge
  - Low-rank (tensor) representations
  - **Sparse learning, (Bayesian) compressive sensing**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
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Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
  - UQ studies seriously hindered
  - Need surrogates with few model simulations
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
- Intrinsic Stochasticity
- **Model Errors**
- Input Correlations
- Low-Probability (Tail) Events
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Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
  - Polynomial representation not good enough
  - Quadrature integration fails

  - Stochastic domain decomposition
  - Data clustering/classification
- Scarce Data
- Intrinsic Stochasticity
- **Model Errors**
- Input Correlations
- Low-Probability (Tail) Events
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Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
  - Bayesian inference is prior-dominated
  - Lack of parameter identifiability
  - Bayesian methods do quantify lack-of-data uncertainty
- Intrinsic Stochasticity
- **Model Errors**
- Input Correlations
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Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
- Intrinsic Stochasticity
  - Quadrature and sparse quadrature methods fail
  - Averaged quantities
  - Bayesian regression
- **Model Errors**
- Input Correlations
- Low-Probability (Tail) Events
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Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
- Intrinsic Stochasticity
- **Model Errors**
  - Models are not perfect
  - Can not be ignored during parameter estimation
  - Additive model error as a Gaussian Process
  - **Embedded model error**
- Input Correlations
- Low-Probability (Tail) Events
- Time Dynamics

Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
- Intrinsic Stochasticity
- **Model Errors**
- Input Correlations
  - Hard to sample from
  - Hard to interpret sensitivities
  - Rosenblatt transformation
- Low-Probability (Tail) Events
- Time Dynamics

Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
- Intrinsic Stochasticity
- **Model Errors**
- Input Correlations
- Low-Probability (Tail) Events
  - PC inaccurate in capturing regions of low probability
  - Use targeted PC germs ξ with fat tails
- Time Dynamics

Laundry List of Challenges/Issues (incomplete)

- **High-Dimensionality**
- Expensive Models
- Non-Linear Models, Discontinuities, Bimodalities
- Scarce Data
- Intrinsic Stochasticity
- **Model Errors**
- Input Correlations
- Low-Probability (Tail) Events
- Time Dynamics
  - Large amplification of phase errors over long time horizon
  - Chaotic dynamics

  - Increase order with time to retain accuracy
  - Ad-hoc corrections
  - Look at averaged quantities

Outline

Surrogate construction: scope and challenges

Construct surrogate for a complex model $f(\boldsymbol{\lambda})$ to enable

- Global sensitivity analysis
- Optimization
- Forward uncertainty propagation
- Input parameter calibration
- $\cdots$

- Computationally expensive model simulations, data sparsity
  - Need to build accurate surrogates with as few training runs as possible
- High-dimensional input space
  - Too many samples needed to cover the space
  - Too many terms in the polynomial expansion

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Alternative methods to obtain PC coefficients

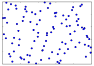
$$Z = f(U(\boldsymbol{\xi})) \simeq \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi})$$

- Projection $\qquad f_k = \frac{\langle f(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \rangle}{||\Psi_k||^2}$

  The integral $\langle f(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \rangle = \int f(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \pi_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}$ is estimated by...

  - Monte-Carlo

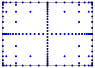
$$\frac{1}{N} \sum_{j=1}^{N} f(\boldsymbol{\xi}_j) \Psi_k(\boldsymbol{\xi}_j)$$



many(!) random samples

  - Quadrature

$$\sum_{j=1}^{Q} f(\boldsymbol{\xi}_j) \Psi_k(\boldsymbol{\xi}_j) w_j$$



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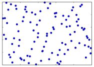

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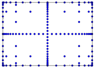
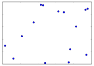


samples at quadrature

- Bayesian regression

$$P(f_k|f(\boldsymbol{\xi}_j)) \propto P(f(\boldsymbol{\xi}_j)|f_k)P(f_k)$$



any (number of) samples

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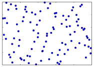

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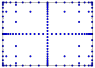

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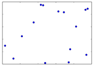
- Bayesian regression

$$\underbrace{P(\boldsymbol{f}|\mathcal{D})}_{\text{Posterior}} \propto \underbrace{P(\mathcal{D}|\boldsymbol{f})}_{\text{Likelihood}}\underbrace{P(\boldsymbol{f})}_{\text{Prior}}$$



any (number of) samples

Bayesian inference of PC surrogate

$$Z = f(\boldsymbol{\xi}) \simeq \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi}) \equiv f_s(\boldsymbol{\xi}) \qquad \overbrace{P(\boldsymbol{f}|\mathcal{D})}^{\text{Posterior}} \propto \overbrace{P(\mathcal{D}|\boldsymbol{f})}^{\text{Likelihood}} \overbrace{P(\boldsymbol{f})}^{\text{Prior}}$$

- Data consists of *training runs*

$$\mathcal{D} \equiv \{(\boldsymbol{\xi}_i, Z_i)\}_{i=1}^{N}$$

- Likelihood with a gaussian noise model with σ^2 fixed or inferred,

$$L(\boldsymbol{f}) = P(\mathcal{D}|\boldsymbol{f}) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} \exp\left(-\frac{(f_i - f_s(\boldsymbol{\xi}_i))^2}{2\sigma^2}\right)$$

- Prior on $\boldsymbol{f}$ is chosen to be conjugate, uniform or gaussian.
- Posterior is a *multivariate normal*

$$\boldsymbol{f} \quad \in \quad \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

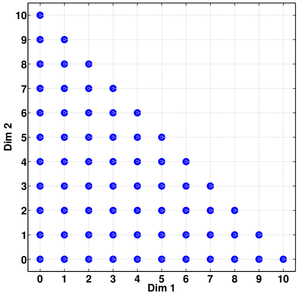
- The (uncertain) surrogate is *a gaussian process*

$$f_s(\boldsymbol{\xi}) = \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi}) = \boldsymbol{\Psi}(\boldsymbol{\xi})^T \boldsymbol{f} \quad \in \quad \mathcal{GP}(\boldsymbol{\Psi}(\boldsymbol{\xi})^T \boldsymbol{\mu}, \boldsymbol{\Psi}(\boldsymbol{\xi})\boldsymbol{\Sigma}\boldsymbol{\Psi}(\boldsymbol{\xi}')^T)$$

Bayesian inference of PC surrogate: high-d, low-data regime

$$Z = f(\boldsymbol{\xi}) \approx \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi})$$

$$\Psi_k(\xi_1, \xi_2, ..., \xi_d) = \psi_{k_1}(\xi_1)\psi_{k_2}(\xi_2)\cdots\psi_{k_d}(\xi_d)$$



- Issues:
  - how to properly choose the basis set?
  - need to work in underdetermined regime $N < K$: fewer data than bases (d.o.f.)

- Discover the underlying low-d structure in the model
  - get help from the machine learning community

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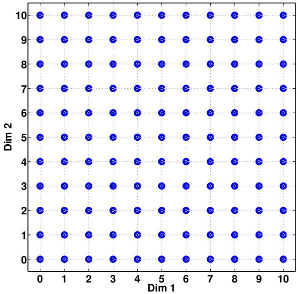

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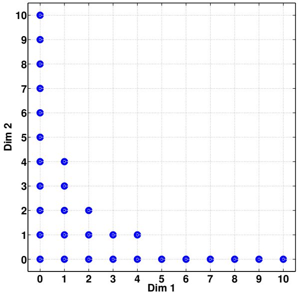

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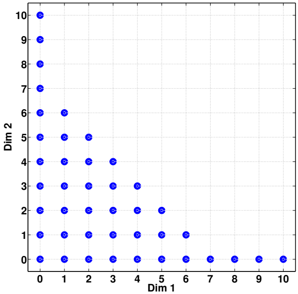

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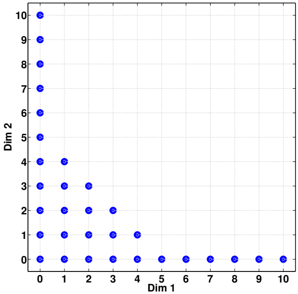

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In a different language....

- N training data points $(\boldsymbol{\xi}_i, Z_i)$ and $K+1$ basis terms $\Psi_k(\cdot)$
- Projection matrix $\boldsymbol{P}^{N\times(K+1)}$ with $\boldsymbol{P}_{ik} = \Psi_k(\boldsymbol{x}_i)$
- Find regression weights $\boldsymbol{f} = (f_0, \ldots, f_K)$ so that

$$\boldsymbol{Z} \approx \boldsymbol{P}\boldsymbol{f} \quad \text{or} \quad Z_i \approx \sum_{k=0}^{K} f_k \Psi_k(\boldsymbol{\xi}_i)$$

- The number of polynomial basis terms grows fast; a p-th order, d-dimensional basis has a total of $K+1 = (p+d)!/(p!d!)$ terms.
- For limited data and large basis set ($N \leq K$) this is a sparse signal recovery problem $\Rightarrow$ need some regularization/constraints.

- Least-squares $\quad \mathit{argmin}_{\boldsymbol{c}} \{||\boldsymbol{Z} - \boldsymbol{P}\boldsymbol{f}||_2\}$
- The ‘sparsest’ $\quad \mathit{argmin}_{\boldsymbol{c}} \{||\boldsymbol{Z} - \boldsymbol{P}\boldsymbol{f}||_2 + \alpha||\boldsymbol{f}||_0\}$
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Bayesian $\quad$ Likelihood $\quad$ Prior

Bayesian Compressive Sensing (BCS), or Relevance Vector Machine (RVM)

- Dimensionality reduction by using hierarchical priors

$$p(f_k|\sigma_k^2) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{f_k^2}{2\sigma_k^2}} \qquad p(\sigma_k^2|\alpha) = \frac{\alpha}{2} e^{-\frac{\alpha\sigma_k^2}{2}}$$

- Effectively, one obtains Laplace *sparsity* prior

$$p(\boldsymbol{f}|\alpha) = \int \prod_{k=0}^{K-1} p(f_k|\sigma_k^2)p(\sigma_k^2|\alpha)d\sigma_k^2 = \prod_{k=0}^{K-1} \frac{\sqrt{\alpha}}{2} e^{-\sqrt{\alpha}|f_k|}$$

- The parameter α can be further modeled hierarchically, or fixed.
- Evidence maximization dictates values for $\sigma_k^2, \alpha, \sigma^2$ and allows exact Bayesian solution

$$\boldsymbol{c} \sim \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

with

$$\boldsymbol{\mu} = \sigma^{-2}\boldsymbol{\Sigma}\boldsymbol{P}^T\boldsymbol{u} \qquad \boldsymbol{\Sigma} = \sigma^2(\boldsymbol{P}^T\boldsymbol{P} + \mathrm{diag}(\sigma^2/\sigma_k^2))^{-1}$$

[Tipping, 2001, Ji *et al.*, 2008; Babacan *et al.*, 2010]

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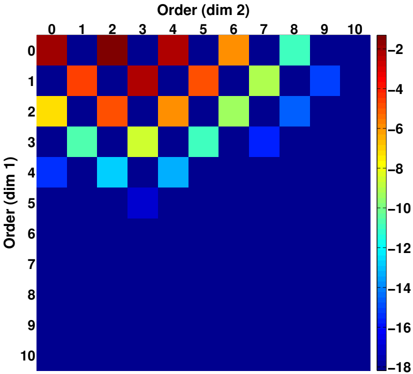
- KEY: Some $\sigma_k^2 \to 0$, hence the corresponding basis terms are dropped.

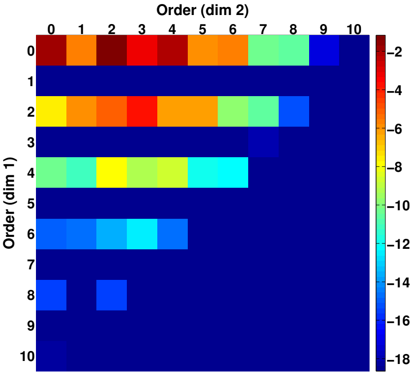
[Tipping, 2001, Ji *et al.*, 2008; Babacan *et al.*, 2010]

BCS removes unnecessary basis terms

$f(x,y) = \cos(x + 4y)$

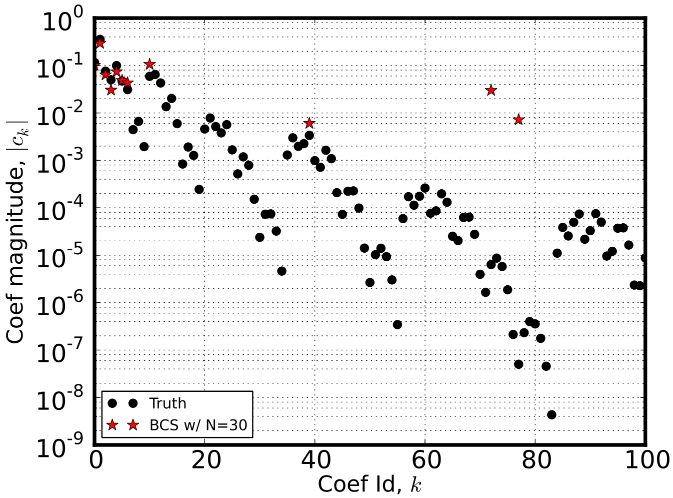


$f(x,y) = \cos(x^2 + 4y)$



The square (i,j) represents the (log) spectral coefficient for the basis term $\psi_i(x)\psi_j(y)$.

BCS recovers true PC coefficients with increased number of measurements



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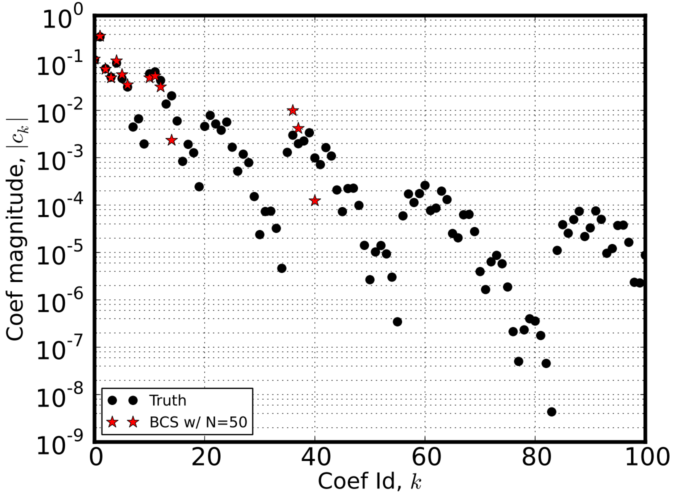

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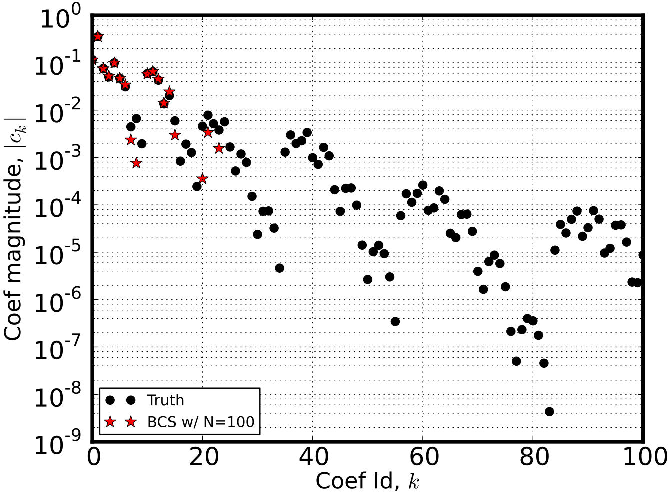

Bayesian Compressive Sensing

- Dimensionality reduction by using hierarchical priors

$$p(f_k|\sigma_k^2) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{f_k^2}{2\sigma_k^2}} \qquad\qquad p(\sigma_k^2|\alpha) = \frac{\alpha}{2} e^{-\frac{\alpha\sigma_k^2}{2}}$$

- Effectively, one obtains Laplace *sparsity* prior

$$p(\boldsymbol{c}|\boldsymbol{\alpha}) = \int \prod_{k=0}^{K-1} p(f_k|\sigma_k^2) p(\sigma_k^2|\alpha) d\sigma_k^2 = \prod_{k=0}^{K-1} \frac{\sqrt{\alpha}}{2} e^{-\sqrt{\alpha}|f_k|}$$

- The parameter α can be further modeled hierarchically, or fixed.
- Evidence maximization dictates values for $\sigma_k^2, \alpha, \sigma^2$ and allows exact Bayesian solution

$$\boldsymbol{f} \sim \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

  with

$$\boldsymbol{\mu} = \sigma^{-2} \boldsymbol{\Sigma} \boldsymbol{P}^T \boldsymbol{u} \qquad\qquad \boldsymbol{\Sigma} = \sigma^2 (\boldsymbol{P}^T \boldsymbol{P} + \mathrm{diag}(\sigma^2/\sigma_k^2))^{-1}$$

- KEY: Some $\sigma_k^2 \to 0$, hence the corresponding basis terms are dropped.

Weighted Bayesian Compressive Sensing

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- KEY: Some $\sigma_k^2 \to 0$, hence the corresponding basis terms are dropped.

Iteratively reweighting Compressive Sensing [Candes *et al.*, 2007]

Sparsest solution:	$min\|\|\boldsymbol{f}\|\|_0$ such that $\boldsymbol{Z} \approx \boldsymbol{P}\boldsymbol{f}$
Compressive sensing:	$min\|\|\boldsymbol{f}\|\|_1$ such that $\boldsymbol{Z} \approx \boldsymbol{P}\boldsymbol{f}$
Weighted compressive sensing:	$min\|\|\boldsymbol{W}\boldsymbol{f}\|\|_1$ such that $\boldsymbol{Z} \approx \boldsymbol{P}\boldsymbol{f}$

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For sparse signals, $\boldsymbol{Z} = \boldsymbol{P}\boldsymbol{f}^s$, with $||\boldsymbol{f}^s||_0 = S < K$, ideal weights are

$$\boldsymbol{W} = diag\left(\frac{1}{|f_k^s|}\right)$$ [i.e., $W_{kk} = +\infty$ if $f_k^s = 0$]

In practice, the true signal coefficients are not known, so...

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In practice, the true signal coefficients are not known, so...

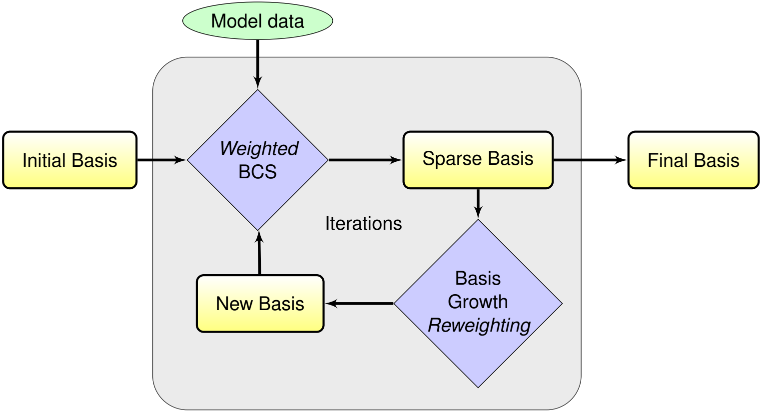
Iterative re-weighting

$$\boldsymbol{W}^{(i+1)} = diag\left(\frac{1}{|f_k^{(i)}| + \epsilon}\right)$$

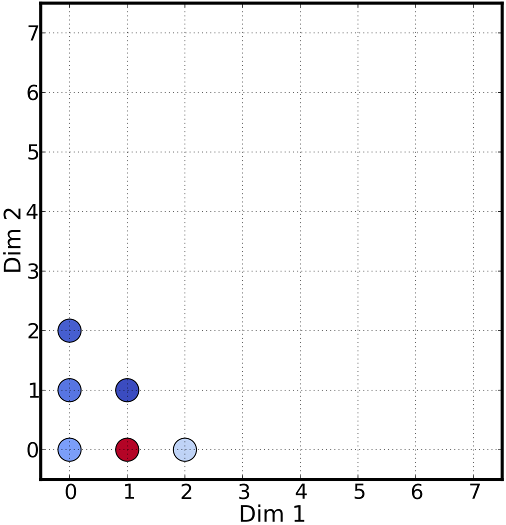
[$\epsilon \ll 1$ for stability]

Weighted Iterative BCS

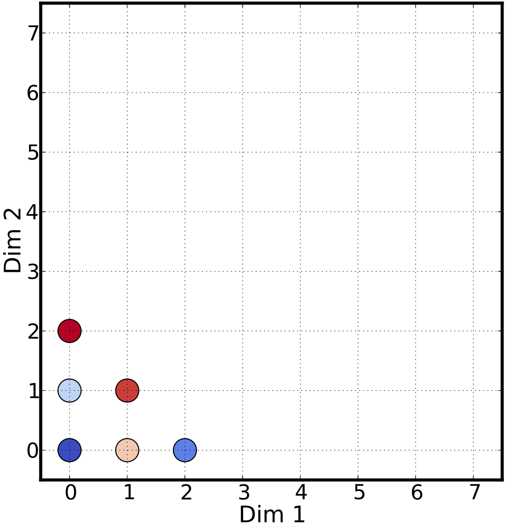
- *Iterative BCS*: We implement an iterative procedure that allows increasing the order for the relevant basis terms while maintaining the dimensionality reduction [Sargsyan *et al.* 2014], [Jakeman *et al.* 2015].
- Combine basis growth and reweighting!



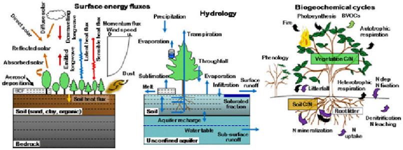
Basis set growth: simple anisotropic function

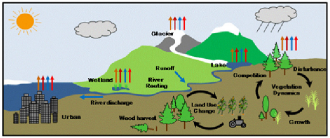


Basis set growth: ... added outlier term



The UQ Challenge for ACME Land Model



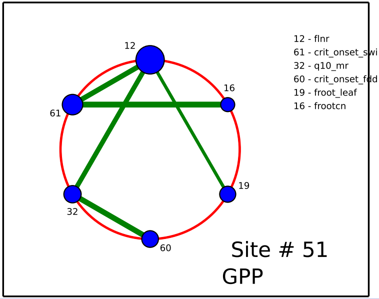


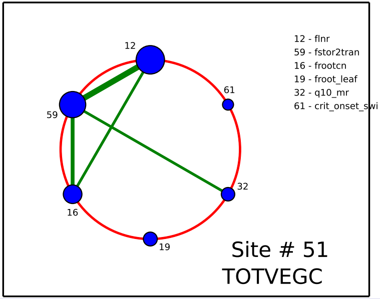
http://www.cesm.ucar.edu/models/clm/

- A single-site, 1000-yr simulation takes ~ 10 hrs on 1 CPU
- Involves ~ 70 input parameters; some dependent
- Non-smooth input-output relationship

Sparse PC surrogate and uncertainty decomposition for the ACME Land Model

- Main effect sensitivities : rank input parameters
- Joint sensitivities : most influential input couplings
- About 200 polynomial basis terms in the 68-dimensional space
- Sparse PC will further be used for
    - sampling in a reduced space
    - parameter calibration against experimental data





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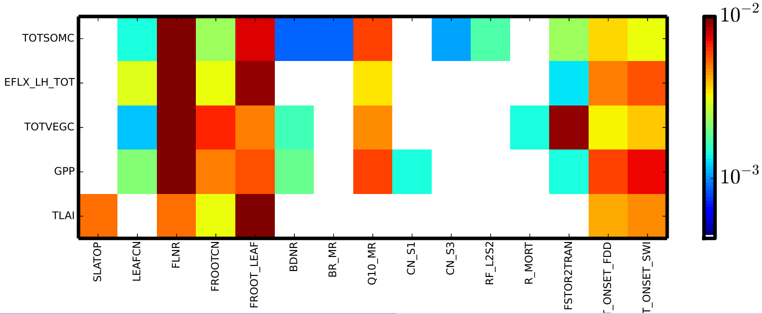

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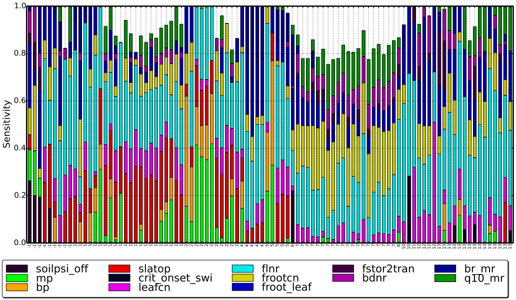
- GPP
  gross primary
  productivity



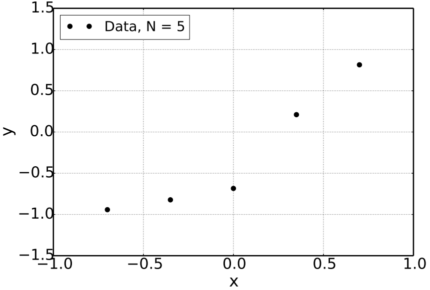
Outline

Main target: quantification of model error

Model error = deviation from 'truth', or from a higher-fidelity model

- Represent and estimate the error associated with
  - Simplifying assumptions, parameterizations
  - Mathematical formulation, theoretical framework
  - Numerical discretization
- ...will be useful for
  - Model validation
  - Model comparison
  - Scientific discovery and model improvement
  - Reliable computational predictions
- Inverse modeling context
  - Given experimental or higher-fidelity model data, estimate the model error

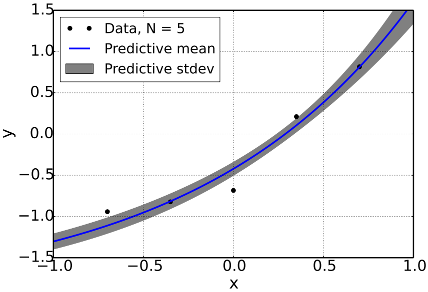
Motivation: can't afford ignoring model error



Model-data fit

- Given noisy data – Gaussian noise
- $y = g_{\text{true}}(x) + \epsilon$

Motivation: can't afford ignoring model error



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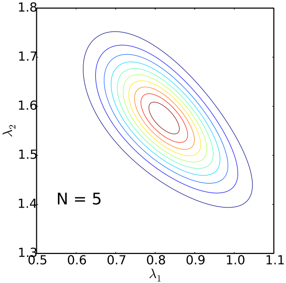

Posterior on parameters

- Employ Bayesian inference to fit an exponential model: $y_{\rm m} = f(x;\lambda)$
- Discrepancy between data and prediction presumed exclusively due to *i.i.d.* Gaussian data noise: $y = f(x;\lambda) + \epsilon_{\rm d}$
- Plotted:
  - Posterior density on the parameters
  - Preditive mean and standard deviation

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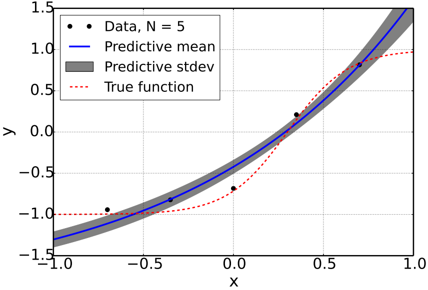

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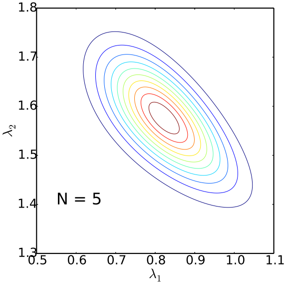

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- True model $g(x)$ – dashed-red – differs from fit model $f(x,\lambda)$
- Actual discrepancy includes both data and model errors

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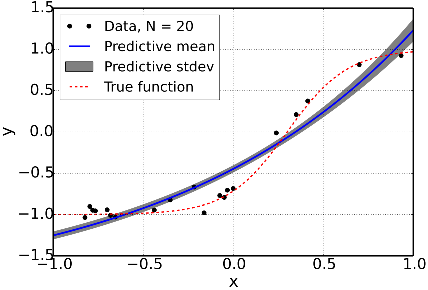

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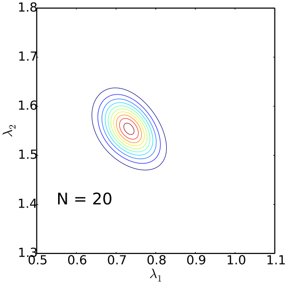

Posterior on parameters

- Increasing number of data points decreases posterior and predictive uncertainty
- We are increasingly sure about predictions based on the *wrong* model

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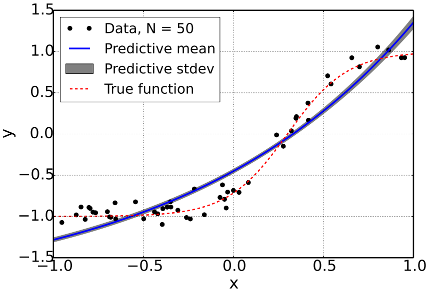

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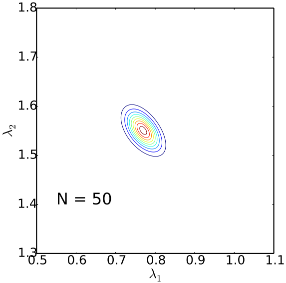

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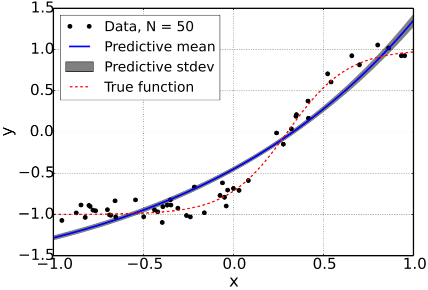

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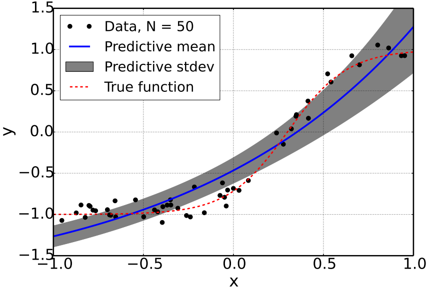


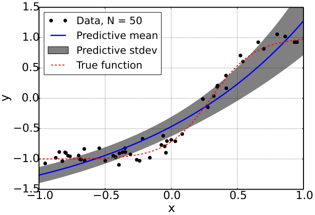
What we want

- If the model has structural uncertainty, more data leads to biased and overconfident results
- We want to quantify model-vs-truth discrepancy in a rigorous and systematic way
  - Cannot ignore model error

Model Error – Challenges with current methods

Total error budget

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



- Ignoring model error $\delta(x)$ leads to incorrect predictive errors
- Conventional statistical modeling (Kennedy and O'Hagan, 2001)
  - makes it difficult to disambiguate model/data errors
  - may violate physical constraints
  - not meaningful for prediction of other QoIs
- Issue is highlighted in model-to-model calibration ($\epsilon_i = 0$)
  - no a priori knowledge of the statistical structure of the discrepancy

Model Error – Key idea: probabilistic embedding

Cast input parameters λ as a random variable Λ

$$y_i = f(x_i;\lambda) + \delta(x_i) + \epsilon_i \longrightarrow y_i = f(x_i;\Lambda) + \epsilon_i$$

- Embed model error in specific submodel phenomenology
  - a modified transport or constitutive law
  - a modified formulation for a material property
  - turbulent model constants
- 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
- Naturally preserves model structure and physical constraints
- Disambiguates model/data errors

Model Error – Bayesian density estimation

$$y_i = f(x_i; \Lambda) + \epsilon_i$$

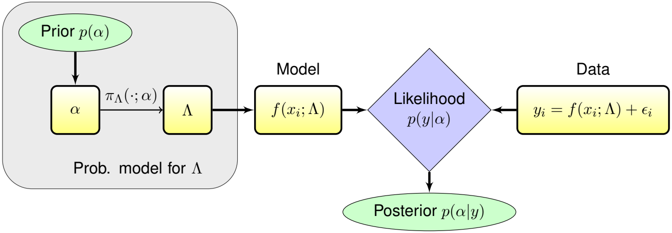
- Parametrise embedded random variable Λ:
  - PDF form $\pi_\Lambda(\cdot; \alpha)$
  - Polynomial Chaos (PC): $\Lambda = \sum_k \alpha_k \Psi_k(\xi)$
  - Multivariate Normal (MVN): $\begin{cases} \Lambda_1 = \alpha_{10} + \alpha_{11}\xi_1 \\ \Lambda_2 = \alpha_{20} + \alpha_{21}\xi_1 + \alpha_{22}\xi_2 \\ \quad\vdots \\ \Lambda_d = \alpha_{d0} + \alpha_{d1}\xi_1 + \alpha_{d2}\xi_2 + \cdots + \alpha_{dd}\xi_d \end{cases}$

- Inverse modeling context
  - Parameter estimation of $\lambda \Rightarrow$ PDF estimation of $\Lambda \Rightarrow$
    $\Rightarrow$ parameter estimation of α
  - Bayesian formulation

$$\underbrace{p(\alpha|y)}_{\text{Posterior}} \propto \underbrace{L_y(\alpha)}_{\text{Likelihood}} \underbrace{p(\alpha)}_{\text{Prior}}$$

Model Error – Likelihood options

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



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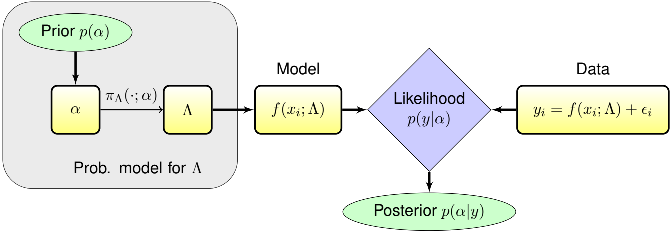

- Full Likelihood: $L(\alpha) = p(y|\alpha) = p(y_1, \ldots, y_N|\alpha) = \pi(y)$
  - Degenerate if no data noise
  - Requires multivariate KDE or high-d integration
  - Gaussian approximation:
    $L(\alpha) \propto \exp\left(-\frac{1}{2}(y - \mu(\alpha))^T \Sigma^{-1}(\alpha)(y - \mu(\alpha))\right)$
  - NISP PC relieves the expense and provides easy access to mean $\mu(\alpha)$ and covariance $\Sigma(\alpha)$

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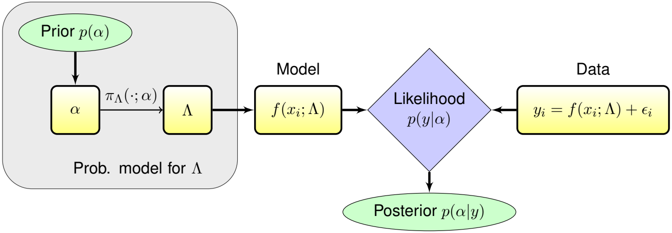

- Marginalized Likelihood: $L(\alpha) = p(y|\alpha) \approx \prod_{i=1}^N p(y_i|\alpha) = \prod_{i=1}^N \pi(y_i)$
  - Requires univariate KDE
  - Neglects built-in correlations
  - Gaussian approximation:
    $L(\alpha) \propto \exp\left(-\frac{1}{2}\sum_{i=1}^N \Sigma_{ii}^{-1}(\alpha)(y_i - \mu_i(\alpha))^2\right)$

Model Error – Likelihood options

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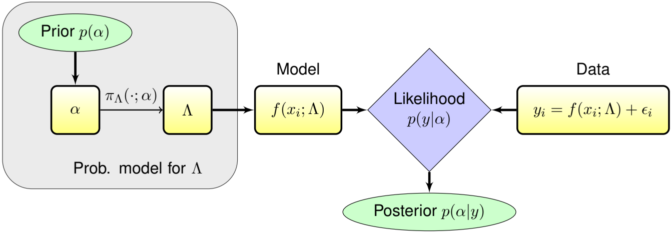


- Approximate Bayesian Computation (ABC): $L(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S}_\mathcal{M},\mathcal{S}_\mathcal{D})}{\epsilon}\right)$
  - Mean of $f(x_i;\Lambda)$ is "centered" on the data
  - The width of the distribution of $f(x_i;\Lambda)$ is consistent with the spread of the data around the nominal model prediction

$$L(\alpha) \propto \exp\left(-\frac{1}{2\epsilon^2}\sum_{i=1}^{N}\left[(\mu_i(\alpha)-y_i)^2 + \left(\sqrt{\Sigma_{ii}(\alpha)} - \gamma|\mu_i(\alpha)-y_i|\right)^2\right]\right)$$

Model Error – Predictions

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

- Non-intrusive spectral projection (NISP) will be employed for
  - Likelihood computation
  - Posterior/pushed-forward predictions
  - Easy access to first two moments:

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

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

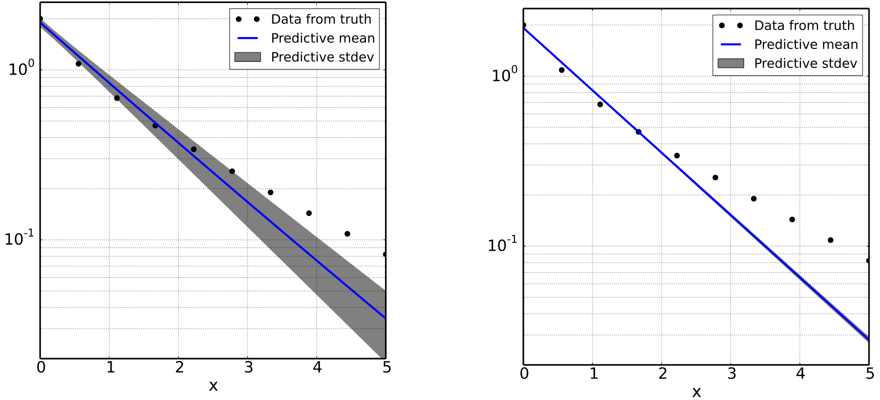
$$\mathbb{V}[y(x)] = \underbrace{\mathbb{E}_\alpha[\sigma^2(x;\alpha)]}_{\text{Model error}} + \underbrace{\mathbb{V}_\alpha[\mu(x;\alpha)] + \sigma_d^2}_{\text{Poserior/Data error}}$$

Predictions account for model error

Calibrating single-exponential models
with data from a double exponential model $g(x) = e^{-0.5x} + e^{-2x}$

Linear-exponential $f(x,\lambda) = e^{\lambda_1 + \lambda_2 x}$

Additive Gaussian error



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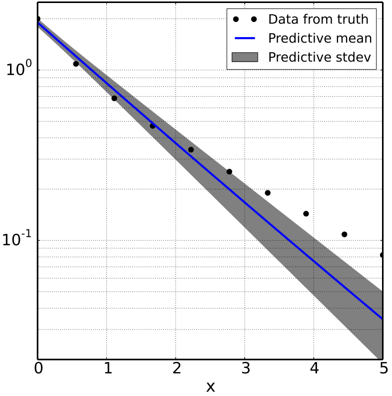
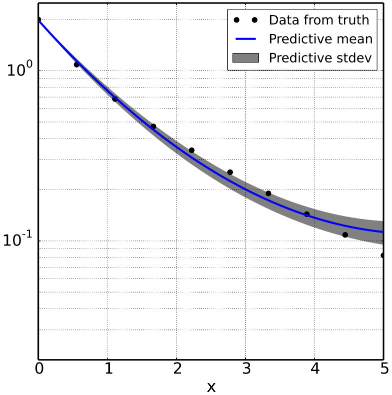


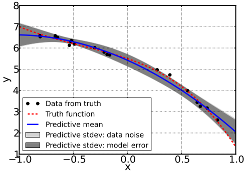
Quadratic-exponential $f_2(x, \lambda) = e^{\lambda_1 + \lambda_2 x + \lambda_3 x^2}$



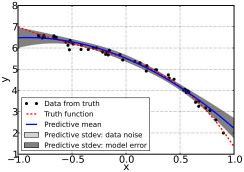
More data leads to ‘leftover’ model error

Calibrating a quadratic $f(x) = \lambda_0 + \lambda_1 x + \lambda_2 x^2$
w.r.t. ‘truth’ $g(x) = 6 + x^2 - 0.5(x+1)^{3.5}$ measured with noise $\sigma = 0.1$.

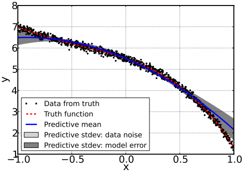
$N = 20$



$N = 50$

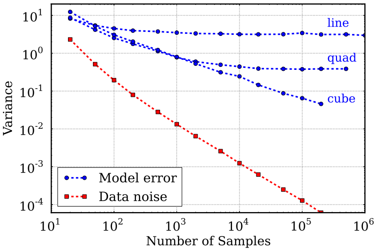


$N = 1000$



Summary of features:

- Well-defined model-to-model calibration
- Model-driven discrepancy correlations
- Respects physical constraints
- Disambiguates model and data errors
- Calibrated predictions of multiple QoIs



Chemistry problem – ABC

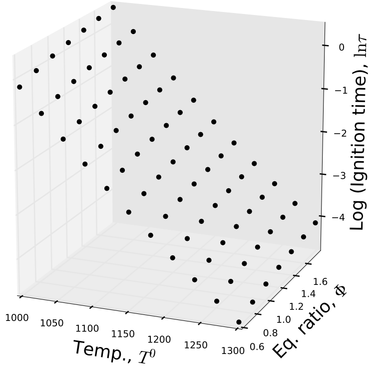
- Homogeneous ignition, methane-air mixture
- Single-step global reaction model calibrated against a detailed chemical kinetic model

- Data: ignition time; range of initial T & equivalence ratio
- Single-step model:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$\begin{aligned} \mathfrak{R} &= [CH_4][O_2]k_f \\ k_f &= A\exp(-E/R^oT) \end{aligned}$$

- $(\ln A, E) = \sum_k \boldsymbol{\alpha}_k \Psi_k(\boldsymbol{\xi})$

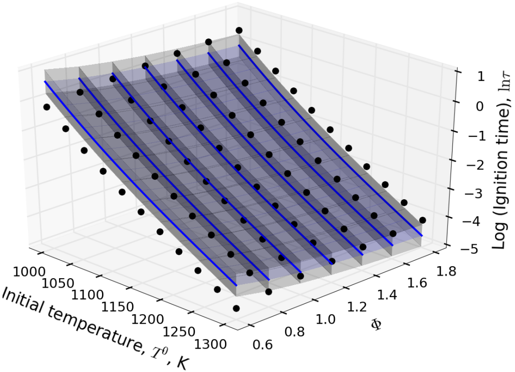


Quality of Uncertain Calibrated Model Predictions

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

TransCom3 Experiment of CO_2 Flux Inversion

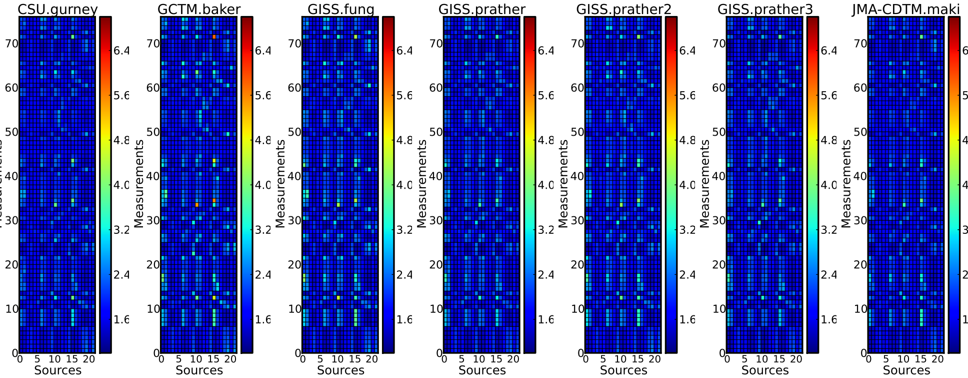
[Gurney *et al.*, Tellus B, 2003]

- Observations $\mathbf{d}$ at $N = 77$ sites around the world
- Inverse problem: find fluxes $\mathbf{s}$ at $M = 22$ locations
- Linearized 'response' model $\mathbf{R}$, such that $\mathbf{d} \approx \mathbf{R}\mathbf{s}$

$$\mathbf{d} = \mathbf{R}\mathbf{s} + \boldsymbol{\epsilon}_\mathbf{d}$$

- Model $\mathbf{R}$ is never perfect thus contaminating the inversion
- The inferred values of $\mathbf{s}$ compensate for model deficiencies
- $\boldsymbol{\epsilon}_\mathbf{d}$ is meant to capture data errors, but is 'entangled' with model errors

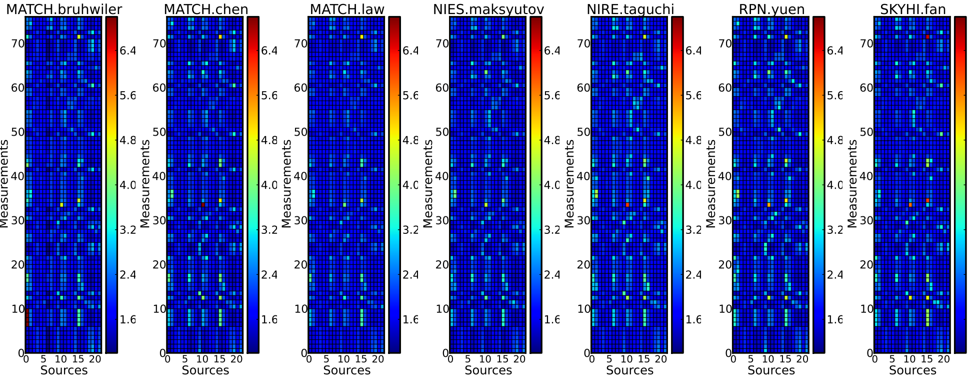
Consider 14 different response models $\mathbf{R}$



Infer fluxes $\mathbf{s}$, given measurements $\mathbf{d}$ to satisfy $\mathbf{d} \approx \mathbf{R}\mathbf{s}$

- Conventional additive Gaussian error (least-squares): $\mathbf{d} = \mathbf{R}\mathbf{s} + \xi$
- Embed probabilistic model for fluxes s: $\mathbf{d} = \mathbf{R}(\mu_\mathbf{s} + \mathbf{C}_\mathbf{s}\xi)$

Consider 14 different response models $\mathbf{R}$



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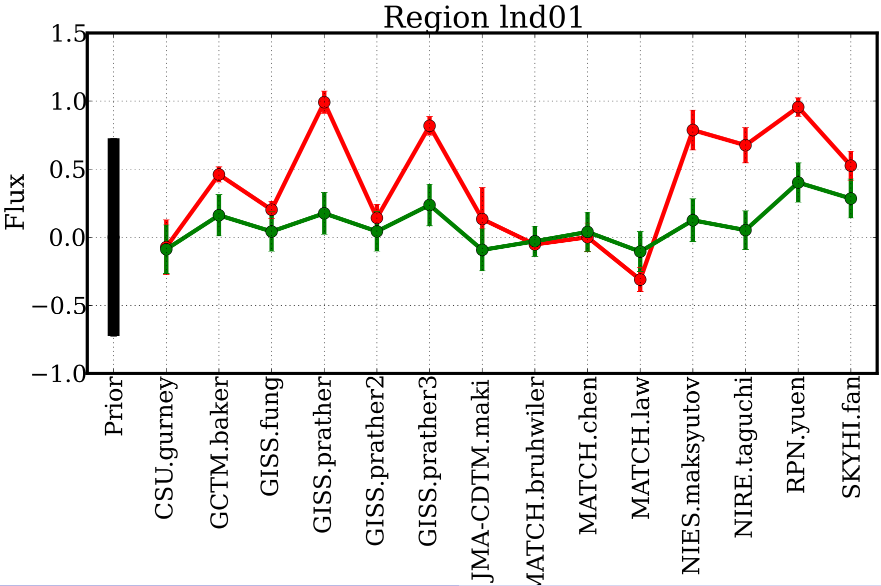
Inferred fluxes show less variability across models



Inferred fluxes show less variability across models

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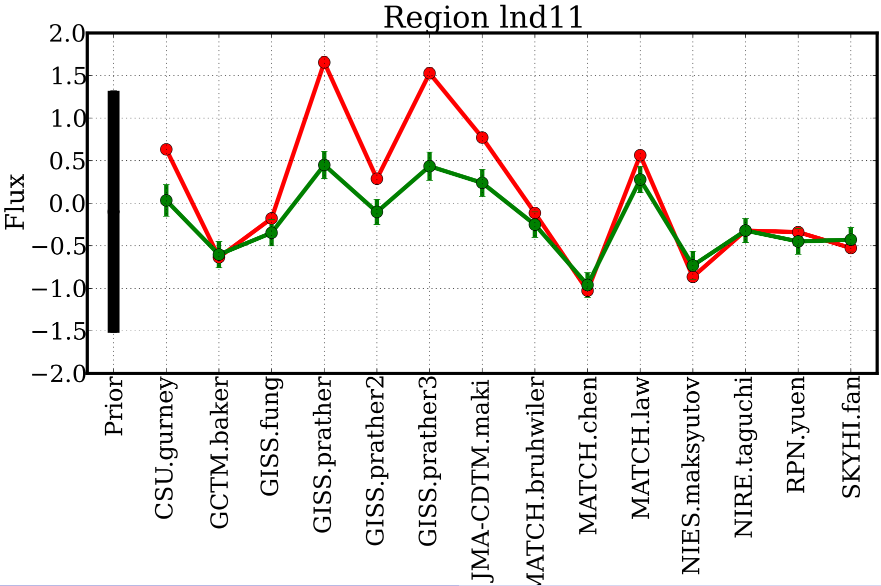
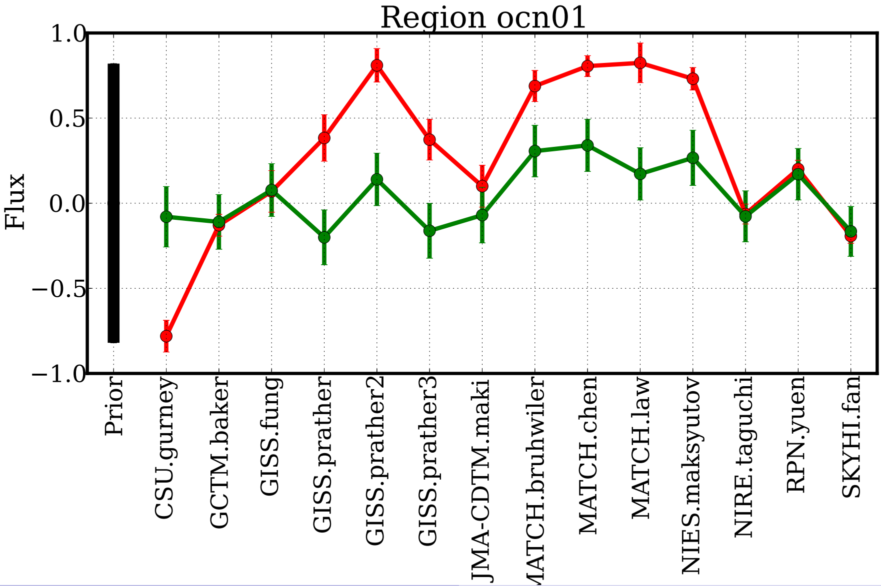


Inferred fluxes show less variability across models



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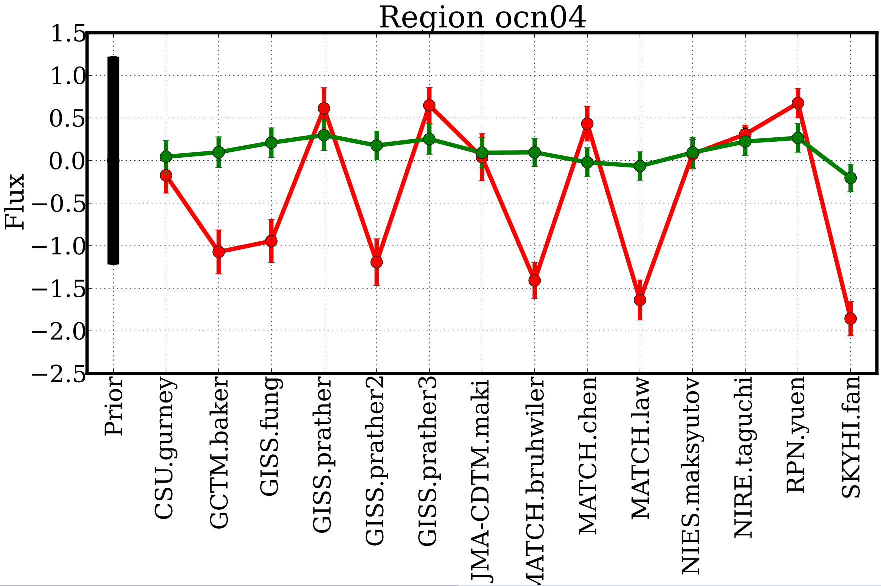

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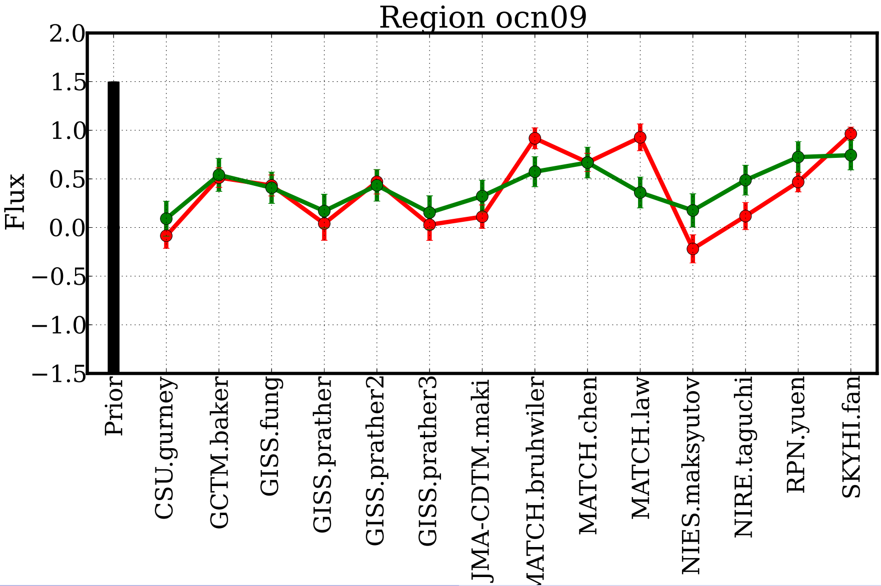
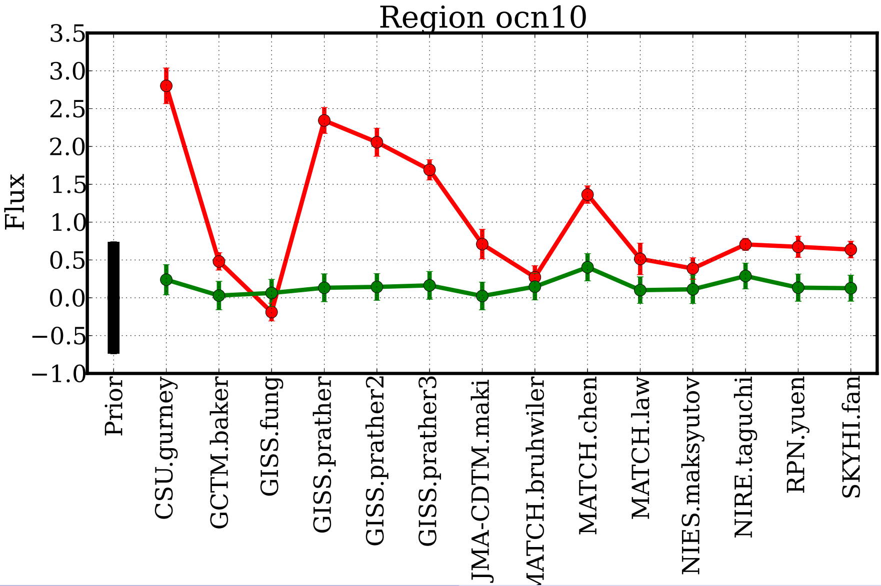


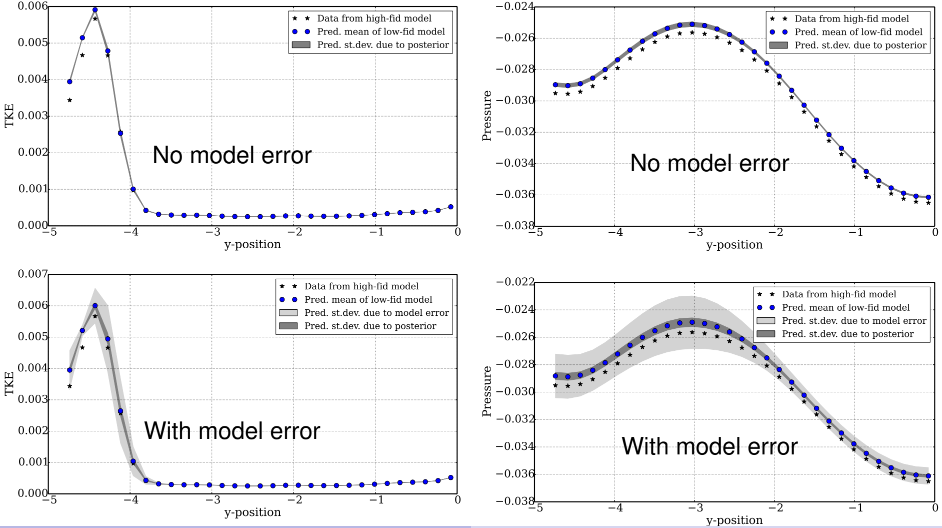
Inferred fluxes show less variability across models



Model error in LES: embed model err in Smagorinsky coefficient
Calibrate with TKE data, predict both TKE and Pressure

Pushed forward posterior

TKE Pressure



Summary

- Forward UQ: Polynomial Chaos representation of RVs
  - Non-intrusive spectral projection
  - Surrogate construction, Bayesian regression
  - **High-D challenge: sparse PC via Bayesian compressive sensing**

- Intrusive spectral projection
- Time/space-resolved processes (Karhunen-Loeve expansions)
- Non-polynomial regression (Radial Basis Functions, Gaussian Processes)
- Rosenblatt transform, Kernel Density Estimation
- Domain decomposition, multiwavelets

Summary

- Inverse UQ: Bayesian inference for parameter estimation
  - Bayesian parameter estimation
  - **Model error quantification: embedded model error approach**

- Markov chain Monte Carlo (MCMC) details
- Model plausibility theory: evidence, model selection, Bayes factors
- MaxEnt methods, data-free inference

Literature

Thank you!

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Marzouk, Y., Najm, H., “Dimensionality Reduction and Polynomial Chaos Acceleration of Bayesian Inference in Inverse Problems”, *J. Comp. Phys.*, 228(6):1862-1902, (2009).

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K. Sargsyan, H. N. Najm, R. Ghanem, “On the Statistical Calibration of Physical Models”, *Int. J. Chem. Kinetics*, 47(4), 246-276, (2015).

Additional Material (Core Dump)

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

Sensitivity indices are directly computable from PC

$$g(\boldsymbol{\xi}) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

Consider dimensionality $d = 3$, total order $p = 2$,
number of PC terms $P + 1 = (d + p)!/(d!p!) = 10$.

$$g(\xi_1, \xi_2, \xi_3) = c_0 + \ c_1\psi_1(\xi_1) \ + \ c_2\psi_1(\xi_2) \ + \ c_3\psi_1(\xi_3) \ +$$

$$+ \ c_4\psi_2(\xi_1) \ + \ c_5\psi_1(\xi_1)\psi_1(\xi_2) \ + \ c_6\psi_1(\xi_1)\psi_1(\xi_3) \ + \ c_7\psi_2(\xi_2) \ + \ c_8\psi_1(\xi_2)\psi_1(\xi_3) \ + \ c_9\psi_2(\xi_3)$$

Variance contributions

$$Var(g) = 0 + \ c_1^2\langle\psi_1^2\rangle \ + \ c_2^2\langle\psi_1^2\rangle \ + \ c_3^2\langle\psi_1^2\rangle \ +$$

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Joint sensitivities (ξ_1, ξ_2) $\quad (\xi_1, \xi_3)$ $\quad (\xi_2, \xi_3)$

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Variance contributions

$$Var(g) = 0 + \; c_1^2\langle\psi_1^2\rangle \; + \; c_2^2\langle\psi_1^2\rangle \; + \; c_3^2\langle\psi_1^2\rangle \; +$$

$$+ \; c_4^2\langle\psi_2^2\rangle \; + \; c_5^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_6^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_7^2\langle\psi_2^2\rangle \; + \; \boxed{c_8^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle} \; + \; c_9^2\langle\psi_2^2\rangle$$

Joint sensitivities (ξ_1, ξ_2) (ξ_1, ξ_3) $\boxed{(\xi_2, \xi_3)}$

Other non-intrusive methods (stochastic collocation)

- Interpolation: Fit interpolant to samples
  - Oscillation concern in multi-D
- Regression: Estimate best-fit response surface
  - Least-squares
    - Sparsity via ℓ_1 constraints; compressive sensing
  - Bayesian inference
    - Sparsity via Laplace priors; Bayesian compressive sensing
  - Useful when quadrature methods are infeasible, e.g.:
    - Samples given *a priori*
    - Can't choose sample locations
    - Can't take enough samples
    - Forward model is noisy

PCE Construction for Noisy Functions

- Quadrature formulae presume a degree of smoothness
  - No convergence for a noisy function

$$u_k = \frac{1}{\langle \Psi_k^2 \rangle} \int u(\lambda(\boldsymbol{\xi}))\, \Psi_k(\boldsymbol{\xi}) p_{\boldsymbol{\xi}}(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad k = 0, \ldots, P$$

- Sparse-Quadrature formulae are *ill-conditioned* and highly-sensitive to noise
  - No convergence with order
  - Error grows with increased dimensionality
- Options in the presence of noise:
  - RMS fitting for PC coefficients
  - Bayesian inference of PC coefficients

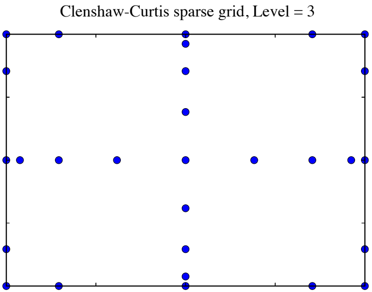
PC and High-Dimensionality

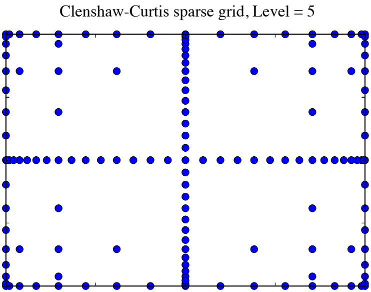
Dimensionality n of the PC basis: $\boldsymbol{\xi} = \{\xi_1, \ldots, \xi_n\}$

- $n \approx$ 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





PC coefficients via sparse regression

PCE:

$$y = f(x) \simeq \sum_{k=0}^{K-1} c_k \Psi_k(x)$$

with $x \in \mathbb{R}^n$, Ψ_k max order p, and $K = (p+n)!/p!/n!$

- N samples $(x_1, y_1), \ldots, (x_N, y_N)$
- Estimate K terms $c_0, \ldots, c_{K-1}$, s.t.

$$\min ||\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}||_2^2$$

where $\boldsymbol{y} \in \mathbb{R}^N$, $\boldsymbol{c} \in \mathbb{R}^K$, $\boldsymbol{A}_{ik} = \Psi_k(x_i)$, $\boldsymbol{A} \in \mathbb{R}^{N \times K}$

With $N << K \Rightarrow$ under-determined

- Need some form of regularization

Regularization – Compressive Sensing (CS)

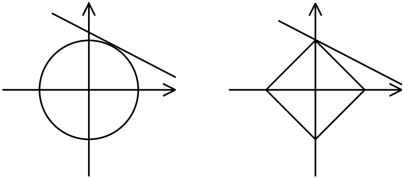
- ℓ_2-norm — Tikhonov regularization; Ridge regression:

$$\min \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \|\boldsymbol{c}\|_2^2\}$$

- ℓ_1-norm — Compressive Sensing; LASSO; basis pursuit

$$\begin{aligned} \min \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \|\boldsymbol{c}\|_1\} & \\ \min \{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2\} & \quad \text{subject to } \|\boldsymbol{c}\|_1 \leq \epsilon \\ \min \{\|\boldsymbol{c}\|_1\} & \quad \text{subject to } \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 \leq \epsilon \end{aligned}$$

$\Rightarrow$ discovery of sparse signals



Bayesian Regression

- Bayes formula
$$p(\boldsymbol{c}|D) \propto p(D|\boldsymbol{c})\pi(\boldsymbol{c})$$
- Bayesian regression: prior as a regularizer, *e.g.*
  - Log Likelihood $\Leftrightarrow$ $\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2$
  - Log Prior $\Leftrightarrow$ $\|\boldsymbol{c}\|_p^p$
- Laplace sparsity priors $\pi(c_k|\alpha) = \frac{1}{2\alpha}e^{-|c_k|/\alpha}$
- LASSO (Tibshirani 1996) ... formally:
$$\min \left\{\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \lambda\|\boldsymbol{c}\|_1\right\}$$
  Solution $\sim$ the posterior mode of $\boldsymbol{c}$ in the Bayesian model
$$y \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{c}, I_N), \qquad c_k \sim \frac{1}{2\alpha}e^{-|c_k|/\alpha}$$
- Bayesian LASSO (Park & Casella 2008)

Bayesian Compressive Sensing (BCS)

- BCS (Ji 2008; Babacan 2010)— hierarchical priors:
  - Gaussian priors $\mathcal{N}(0, \sigma_k^2)$ on the c_k
  - Gamma priors on the σ_k^2

$\Rightarrow$ Laplace sparsity priors on the c_k

- Evidence maximization establishes ML estimates of the σ_k
  - many of which are found $\approx 0 \quad \Rightarrow \quad c_k \approx 0$
  - iteratively include terms that lead to the largest increase in the evidence
- iterative BCS (iBCS) (Sargsyan 2012):
  - adaptive iterative order growth
  - BCS on order-p Legendre-Uniform PC
  - repeat with order-$p+1$ terms added to surviving p-th order terms

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

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

- Given model equations: $\mathcal{M}(u(\boldsymbol{x},t);\lambda)=0$
- 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: $\mathcal{G}(U(\boldsymbol{x},t),\Lambda)=0$
  - with $U=[u_0,\dots,u_P]^T$, $\Lambda=[\lambda_0,\dots,\lambda_P]^T$
- Solving this <u>deterministic</u> system <u>once</u> provides the full specification of uncertain model ouputs

Intrusive Galerkin PC ODE System

$$\boxed{\frac{du}{dt} = f(u;\lambda)}$$

$$\lambda = \sum_{i=0}^{P} \lambda_i \Psi_i \qquad u(t) = \sum_{i=0}^{P} u_i(t)\Psi_i$$

$$\boxed{\frac{du_i}{dt} = \frac{\langle f(u;\lambda)\Psi_i\rangle}{\langle \Psi_i^2 \rangle} \qquad i = 0, \ldots, P}$$

Say $f(u;\lambda) = \lambda u$, then

$$\frac{du_i}{dt} = \sum_{p=0}^{P}\sum_{q=0}^{P} \lambda_p u_q C_{pqi}, \quad i = 0, \cdots, P$$

where the tensor $C_{pqi} = \langle \Psi_p \Psi_q \Psi_i \rangle / \langle \Psi_i^2 \rangle$ is readily evaluated

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 <u>can</u> deliver superior performance

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

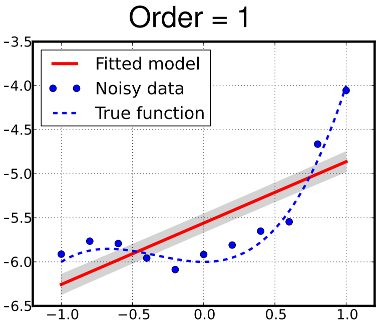
Data model: $i = 1, \dots, N$

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

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

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

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



Fitted model pushed-forward posterior versus the data

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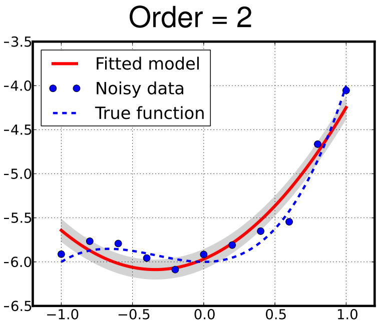

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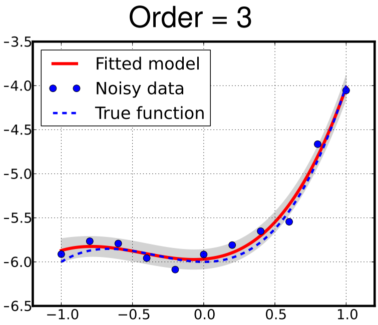

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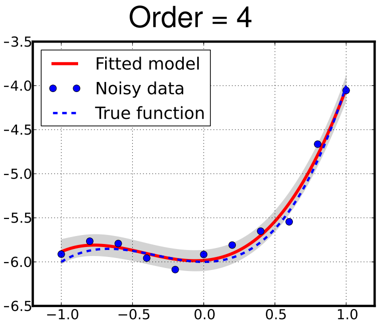

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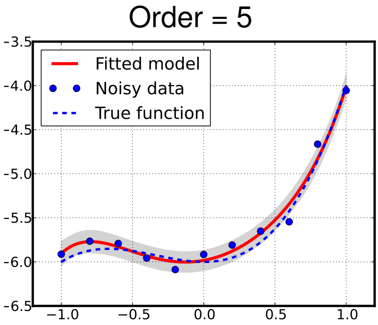

Fitted model pushed-forward posterior versus the data

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\end{aligned}
$$

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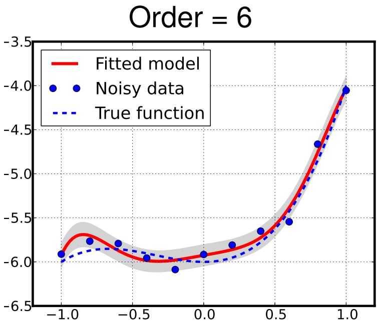

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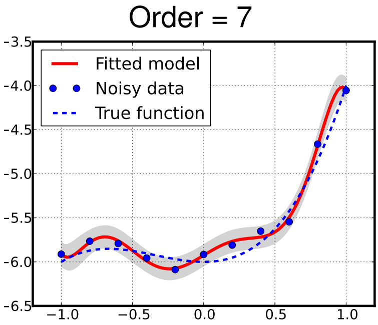

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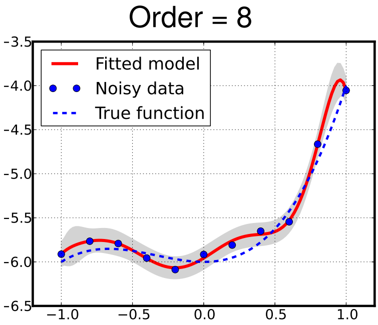

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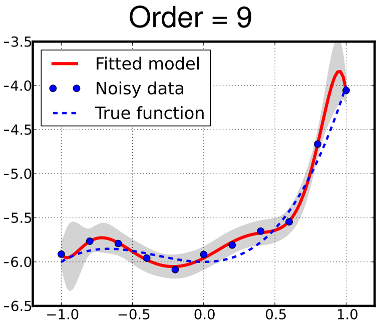

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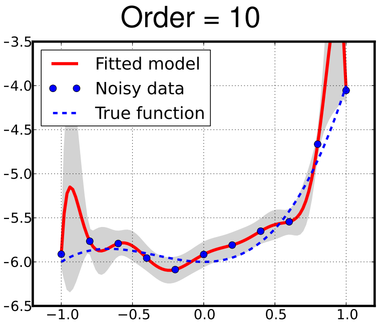
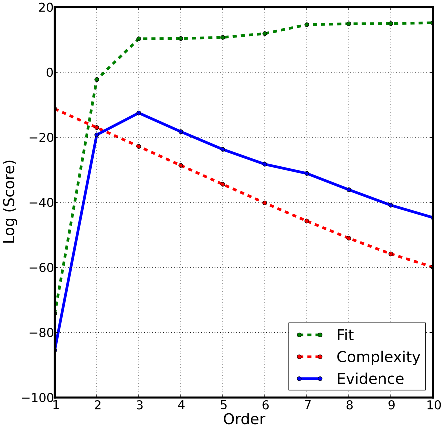


Fitted model pushed-forward posterior versus the data

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



Log evidence: sum of two scores, balances complexity & fit

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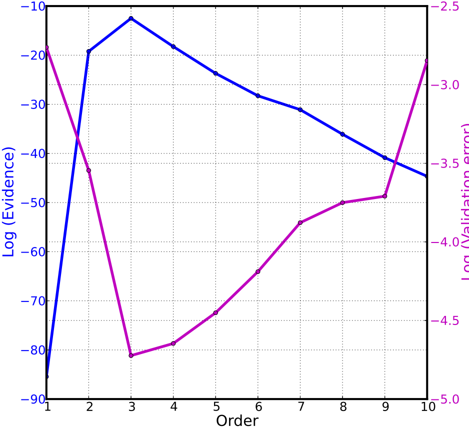

Cross validation error and model evidence versus order

Challenges in PC UQ – High-Dimensionality

- Dimensionality n of the PC basis: $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}$
  - number of degrees of freedom
  - $P + 1 = (n + p)!/n!p!$ grows fast with n
- Impacts:
  - Size of intrusive system
  - # non-intrusive (sparse) quadrature samples
- Generally $n \approx$ number of uncertain parameters
- Reduction of n:
  - Sensitivity analysis
  - Dependencies/correlations among parameters
  - Dominant eigenmodes of random fields
  - Manifold learning: Isomap, Diffusion maps
  - Sparsification: Compressed Sensing, LASSO

High dimensionality challenge – Forward UQ

Consider a forward model

$$y = f(x)$$

Let $x \in \mathbb{R}^n$ be uncertain, represented as a random vector,

$$x \sim p(x)$$

Estimate moments of y

$$\mathcal{M}^q = \int [f(x)]^q p(x) \mathrm{d}x$$

Forward UQ is an integration problem.

Integration in High Dimensions

- Monte Carlo (MC) methods
  - well suited for high-D integrals – convergence rate independent of dimensionality
  - nonetheless they require large numbers of samples for good accuracy
- Quadrature
  - Tensor product quadrature is useless in hi-D
    - Say m points in each of n dimensions: m^n points
  - Adaptive sparse quadrature
    - Much more feasible
    - Can beat MC – dep. on smoothness of integrand
  - Greedy algorithms
- Dimensionality reduction
  - Low rank and sparse representations
  - Global sensitivity analysis

High dimensionality challenge – Inverse UQ

- Bayesian inference in a computational setting relies on Markov Chain Monte Carlo (MCMC) methods
- MCMC: A random walk algorithm for generation of samples from the *posterior* density on model inputs
  - Moments are evaluated from the random samples
- Need many random sample evaluations of forward model
  - Employ model surrogates built via forward UQ
  - *Adaptive local surrogates*
- High dimensionality can lead to poor performance
  - local maxima
  - many directions uninformed by data
  - choice of proposal density
  - *Dimension-Adaptive Likelihood-Informed* MCMC

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)

Curse of Dimensionality

- (Dim-adaptive) Sparse quadrature integration [Gerstner, 2003]
- High Dimensional Model Representation [Rabitz & Alis, 1999]
  - would not handle strong nonlinearities
  - tried cut-HDMR in a chemical kinetics context: fails!
- Proper Generalized Decomposition [Nuoy, 2010]

- Turn it into the *blessing of dimensionality* [Donoho, 2000]
- Compressive sensing in spectral methods [Doostan *et al.*, 2009]
- Bayesian compressive sensing [Ji *et al.*, 2008]

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short answer: no free lunch

Challenges in PC UQ – Non-Linearity

- Bifurcative response at critical parameter values
  - Rayleigh-Bénard convection
  - Transition to turbulence
  - Chemical ignition
- Discontinuous $u(\lambda(\boldsymbol{\xi}))$
  - Failure of global PCEs in terms of smooth $\Psi_k()$
  - $\Leftrightarrow$ failure of Fourier series in representing a step function
- Local PC methods
  - Subdivide support of $\lambda(\boldsymbol{\xi})$ into regions of smooth $u \circ \lambda(\boldsymbol{\xi})$
  - Employ PC with compact support basis on each region
  - A spectral-element vs. spectral construction
  - Domain mapping

Discontinuities/Nonlinearities/Bifurcations

- Stochastic domain decomposition
  - Wiener-Haar expansions,
    Multiblock expansions,
    Multiwavelets, [Le Maître *et al*, 2004,2007]
  - also known as Multielement PC [Wan & Karniadakis, 2009]
- Data domain decomposition [Sargsyan *et al*, 2009,2010]
  - Data clustering, classification
  - Mixture PC expansions

- Adaptive setting helps
- Does not scale with dimensionality
- For expensive models, can not split much
- *Need a 'smart' domain decomposition*

Challenges in PC UQ – Time Dynamics

- Systems with limit-cycle or chaotic dynamics
- Large amplification of phase errors over long time horizon
- PC order needs to be increased in time to retain accuracy
- Time shifting/scaling remedies

- Futile to attempt representation of detailed turbulent velocity field $\boldsymbol{v}(\boldsymbol{x}, t; \lambda(\boldsymbol{\xi}))$ as a PCE
  - Fast loss of correlation due to energy cascade
  - Problem studied in 60's and 70's
- Focus on flow statistics, *e.g.* Mean/RMS quantities
  - Well behaved
  - Argues for non-intrusive methods with DNS/LES of turbulent flow

Model Complexity challenge

- If a single model run is a challenge then UQ is infeasible
- Most physical model output quantities of interest depend on only a "small" number of parameters, however:
  - Global sensitivity analysis itself requires many samples
  - Even after reduction of dimensionality to, say, 5 parameters, O(100) samples may be necessary
- Large number of independent samples
  - ideally suited for HPC
- Multifidelity UQ methods are useful – forward UQ
  - Use combinations of many low-resolution/low-fidelity runs with a few high-resolution/high-fidelity runs
- Parallel MCMC methods – inverse UQ

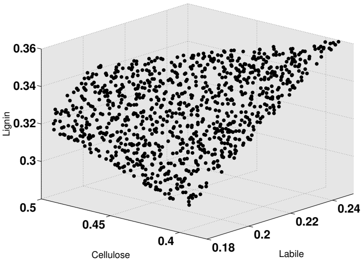
Data Scarcity Challenge

- Even in a “big-Data” context, it’s common to find no information in the data on many *big-model* parameters
  - Situation is typical in statistical inversion for field quantities
  - Bayesian inference of optimal random field constructions
  - Use adaptive MCMC methods that focus on data-informed parameters
- Usually, raw data is not published
  - Published “data” is essentially processed data products, being statistics on
    - the data, or functions of fitted model parameters
  - Use Maximum-Entropy and Approximate Bayesian Computation (ABC) methods – DFI
    - Discover posterior density on model parameters consistent with published statistics

Input correlations: Rosenblatt transformation

- Rosenblatt transformation maps any (not necessarily independent) set of random variables $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_n)$ to uniform i.i.d.'s $\{\eta_i\}_{i=1}^{n}$ [Rosenblatt, 1952].

$$\begin{aligned}
\eta_1 &= F_1(\xi_1) \\
\eta_2 &= F_{2|1}(\xi_2|\xi_1) \\
\eta_3 &= F_{3|2,1}(\xi_3|\xi_2,\xi_1) \\
&\vdots \\
\eta_n &= F_{n|n-1,\ldots,1}(\xi_n|\xi_{n-1},\ldots,\xi_1)
\end{aligned}$$



- Inverse Rosenblatt transformation $\boldsymbol{\xi} = R^{-1}(\eta)$ ensures a well-defined quadrature integration to build PC [Sargsyan *et al.*, 2010]

$$c_k = \langle \boldsymbol{\xi} \Psi_k(\eta) \rangle = \int R^{-1}(\eta) \Psi_k(\eta) d\eta$$

- Caveat: if only samples of $\boldsymbol{\xi}$ are available, the conditional distributions are hard to evaluate accurately.