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Uncertainty Quantification given Discontinuities, Long-tailed Distributions, and Computationally Intensive Models

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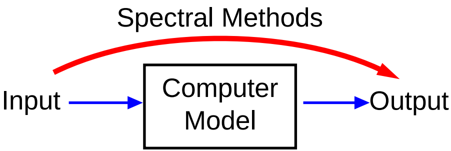
UQ components and methods



Employ sampling-based methods:

- Non-intrusive Spectral Projection (NISP)
- Bayesian Inference

Objective

Tackle two of the challenges encountered in forward UQ:

1. Output observables exhibit discontinuities for smooth changes in the input parameters

2. Model predictions exhibit fat-tailed distributions.

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Expensive Computational Model

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Polynomial Chaos expansion represents random variables as a polynomials of standard random variables

- Truncated PCE: finite dimension n and order p

$$X(\boldsymbol{\lambda}(\boldsymbol{\eta})) \simeq \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\eta})$$

with the number of terms $P + 1 = \frac{(n+p)!}{n!p!}$.

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

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- $\boldsymbol{\eta} = (\eta_1, \cdots, \eta_n)$ standard i.i.d. r.v.
Ψ_k standard orthogonal polynomials
c_k spectral modes.

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- Most common standard Polynomial-Variable pairs:
  Gauss-Hermite, Legendre-Uniform

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

UQ & Discontinuities - Proposed Methodology

Our approach locates the discontinuity first so the domain can be subdivided into regions with smooth model response where spectral uncertainty quantification methods can be used

- Need to represent model output in a problem-independent fashion that takes into account the bifurcations
  - **Bayesian inference of the location of the discontinuity**
- Need to perform uncertainty quantification with only a limited set of sample points, due to the computational cost of the forward model
  - **Polynomial chaos representation via parameter domain mapping**

Bayesian Inference of the Location of Discontinuity

- Parameterize the discontinuity: $\lambda_2 \approx p_{\boldsymbol{c}}(\lambda) = \sum_{k=0}^{K} c_k P_k(\lambda_1)$

- Approximation model:

$$\mathcal{M}_{\boldsymbol{c}} \equiv g(\lambda_1, \lambda_2) = m_L + (m_R - m_L)\frac{1 + \tanh\left(\alpha(\lambda_2 - p_{\boldsymbol{c}}(\lambda_1))\right)}{2}$$

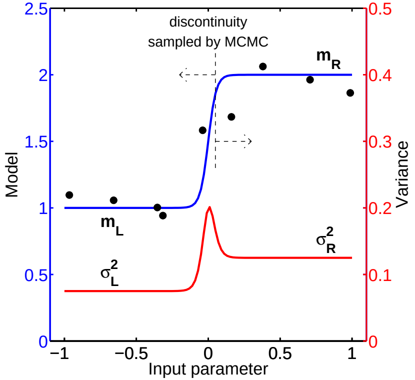
- Noise model postulated: $\sigma(\lambda_1, \lambda_2)$

- Likelihood function:

$$\log P(\mathcal{D}|\mathcal{M}_{\boldsymbol{c}}) = \sum_{i=1}^{N} \log P(z_i|\mathcal{M}_{\boldsymbol{c}}) = -\frac{1}{2}\sum_{i=1}^{N}\left(\frac{(z_i - g_i)^2}{\sigma_i^2} + \log\left(2\pi\sigma_i^2\right)\right)$$

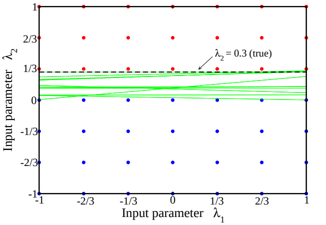
Bayesian Inference of the Location of Discontinuity

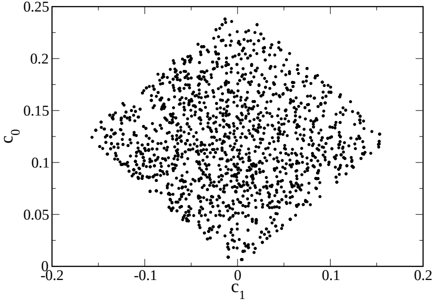
- Parameterize the discontinuity: $\lambda_2 \approx p_{\boldsymbol{c}}(\lambda) = \sum_{k=0}^{K} c_k P_k(\lambda_1)$
- Bayes' formula: $P(\mathcal{M}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{M})P(\mathcal{M})}{P(\mathcal{D})}$

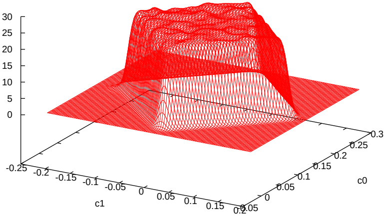


Discontinuity Detection - Highlights

- Any distribution of input points
- Generalizes to multiple dimensions
- Probabilistic representation







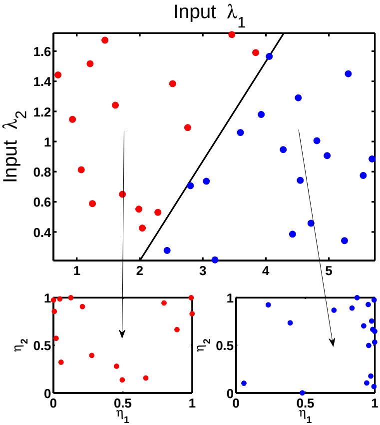
Discontinuity curve samples and their pdf

Parameter Domain Mapping via Rosenblatt Transformation

- Assume linear discontinuity
- Use Rosenblatt Transformation (RT) to map the pair of uncertain parameters (λ_1,λ_2) to i.i.d. uniform random variables η_1 and η_2:

$$\begin{aligned} \lambda_1 &= F_{\lambda}^{-1}(\eta_1), \\ \lambda_2 &= F_{\lambda_2|\lambda_1}^{-1}(\eta_2|\eta_1) \end{aligned}$$

- Apply the RT mapping to both sides of the discontinuity



ROSENBLATT TRANSFORMATION: $(\lambda_1, \lambda_2) \rightarrow (\eta_1, \eta_2)$

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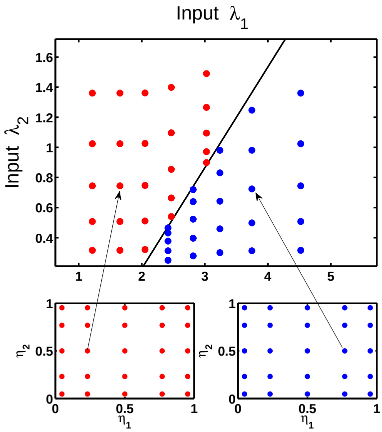

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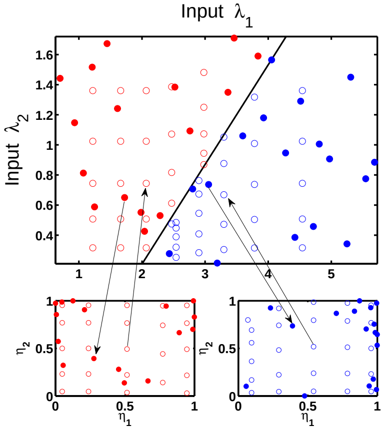

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Compute the Polynomial Chaos Expansions

- PC expansion for the output observable $Z = f(\lambda)$

$$Z \simeq \sum_{k=0}^{K} c_k \Psi_k(\xi)$$

with

$$\langle \Psi_i(\xi)\Psi_j(\xi)\rangle \equiv \int \Psi_i(\xi)\Psi_j(\xi) p_\xi(\xi) d\xi = \delta_{ij}\langle \Psi_i(\xi)^2\rangle$$

- Spectral Projection

$$c_k = \frac{\langle f(\lambda(\xi))\Psi_k(\xi)\rangle}{\langle \Psi_k^2(\xi)\rangle}$$

- Bayesian Inference:

$$P(c_k|f(\lambda_i)) \approx P(f(\lambda_i)|c_k)P(z_k)$$

PC Expansion, Averaged Over Discontinuity Curves

- PC expansion for each discontinuity curve sample:

$$Z_{\boldsymbol{c}}^{L,R}(\vec{\lambda}) = \tilde{Z}_{\boldsymbol{c}}(\vec{\eta}) = \sum_{p=0}^{P} c_p \Psi_p^{(2)}(\vec{\eta})$$

- Model expansion depends on the parameter location:

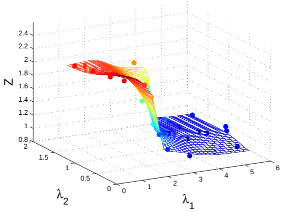
$$Z_{\boldsymbol{c}}(\vec{\lambda}) = \begin{cases} Z_{\boldsymbol{c}}^{L}(\vec{\lambda}) & \text{if } (\vec{\lambda}) \in D_L \\ Z_{\boldsymbol{c}}^{R}(\vec{\lambda}) & \text{if } (\vec{\lambda}) \in D_R \end{cases}.$$

- Average over all PC expansions via RT:

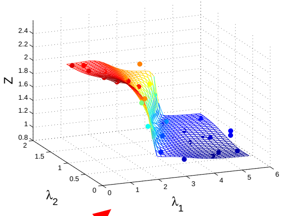
$$\hat{Z}(\vec{\lambda}) = \int_C p(\boldsymbol{c}) Z_{\boldsymbol{c}}(\vec{\lambda}) d\boldsymbol{c} = \int_{[0,1]^{K+1}} Z_{R^{-1}(\vec{\eta})}(\vec{\lambda}) d\vec{\eta}$$

Discontinuous Data Represented Well with the Averaged PC

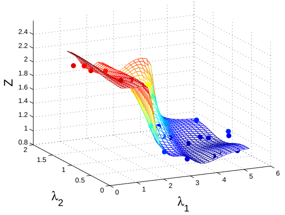
PCE Coefficients via Bayesian Inference

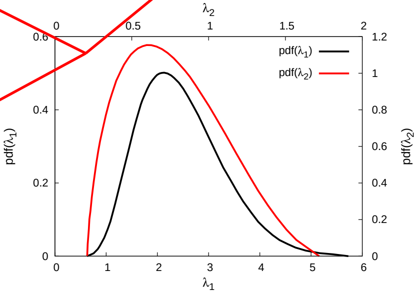


PCE Coefficients via Hybrid Approach



PCE Coefficients via Quadrature Projection





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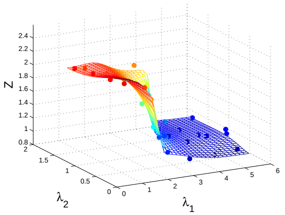
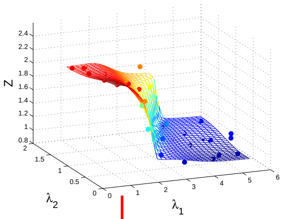
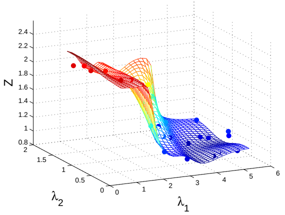
PCE Coefficients via Bayesian Inference

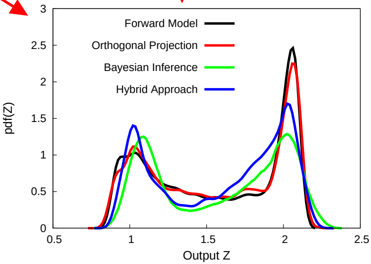


PCE Coefficients via Hybrid Approach



PCE Coefficients via Quadrature Projection



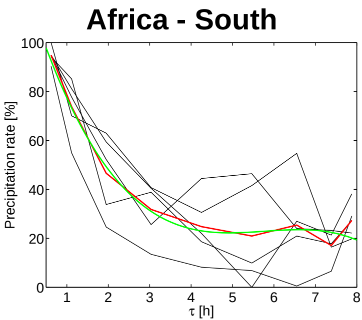


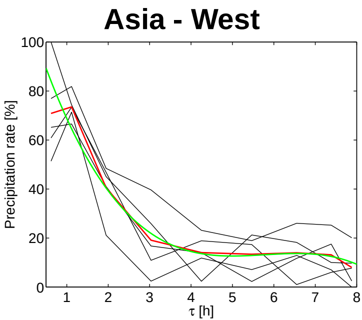
Objective

Tackle two of the challenges encountered in forward UQ:

2. Model predictions exhibit fat-tailed distributions.

Precipitation Data from Climate Simulations



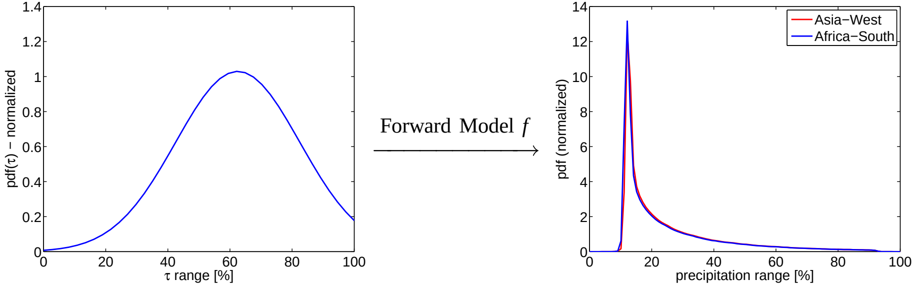


- Precipitation rate scaled between the minimum and maximum encountered in the simulation
- Input parameter τ - consumption rate of CAPE (convective available potential energy)

Black lines - 2 year averages; *Red* lines - 10 year averages; *Green* lines - 3^{rd}-order PC expansions.

(*data courtesy of Mike Levy & Mark Taylor, Sandia National Labs*)

Forward UQ: Input Parameter PDF $\longrightarrow$ Output Observable PDF



- Compute the probability that average precipitation exceeds a certain amount:

$$P(precip. > p_r) = \int_{\tau : f(\tau) > p_r} \text{pdf}(\tau) d\tau$$

Polynomial Chaos Expansions and Galerkin Projection

- PC expansion for the output observable $Z = f(\lambda)$

$$Z \simeq \sum_{k=0}^{K} c_k \Psi_k(\xi)$$

with

$$\langle \Psi_i(\xi)\Psi_j(\xi)\rangle \equiv \int \Psi_i(\xi)\Psi_j(\xi)p_\xi(\xi)d\xi = \delta_{ij}\langle \Psi_i(\xi)^2\rangle$$

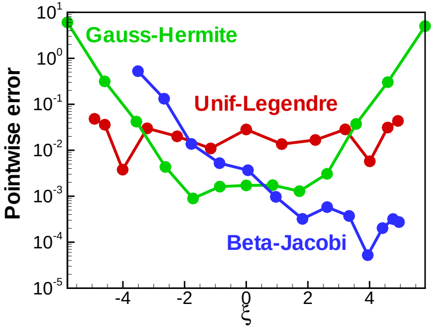
- Galerkin (orthogonal) projection

$$c_k = \frac{\langle f(\lambda(\xi))\Psi_k(\xi)\rangle}{\langle \Psi_k^2(\xi)\rangle}$$

is weighted-L_2 optimal, i.e. it minimizes

$$\int \left| f(\lambda(\xi)) - \sum_{k=0}^{K} c_k \Psi_k(\xi) \right|^2 p_\xi(\xi)d\xi$$

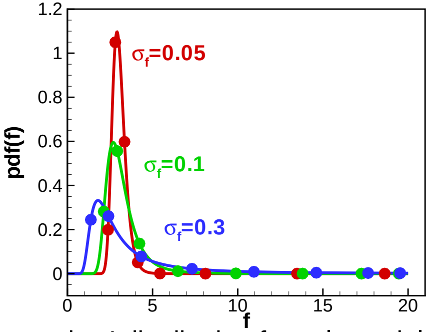
Conventional Basis Functions



- Legendre basis : error is 'independent' of position
- Hermite basis : error is worse in "tails", away from the origin
- Jacobi basis: error is small in desired region, i.e. it is controllable!

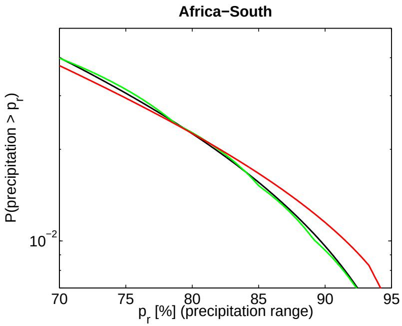
Custom Basis Functions

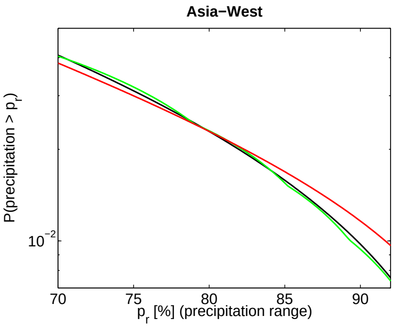
- Design custom polynomials that are orthogonal with respect to fat tailed distributions to get a better accuracy in the tail region.
  - Use Stieltjes or Chebyshev's algorithms. Algorithms are ill-conditioned $\rightarrow$ use arbitrary precision arithmetic software.



(Quadrature points' distribution for polynomials orthogonal w.r.t. truncated log-normal pdf.)

"Tail" Probabilities Based on PC Basis Surrogates





- *Black* lines - "Exact" values; *Red* lines - Hermite PC basis (9^{th} order); *Green* lines - Custom PC basis (9^{th} order).
- The set of quadrature points corresponding to the custom PDF have a better coverage of the distribution's tail compared to the set corresponding to a Gaussian PDF.

Summary and Future Work

- *Nonlinearities, Bifurcations, Bimodalities*
  - Probabilistic detection of discontinuities followed by domain mapping and polynomial chaos expansions to construct model "surrogates"
  - Extend this approach to incorporate optimal experimental design, i.e. find parameter values at which the model should be simulated to give maximum information

Summary and Future Work

- *Nonlinearities, Bifurcations, Bimodalities*
  - Probabilistic detection of discontinuities followed by domain mapping and polynomial chaos expansions to construct model “surrogates”
  - Extend this approach to incorporate optimal experimental design, i.e. find parameter values at which the model should be simulated to give maximum information
- *Tail regions*
  - Construct custom spectral basis based on “expected” shape of the computer model output to improve convergence of the spectral expansion.
  - Extend this methodology to multi-dimensional parameter dependencies.
  - Develop surrogate models as mixed PC expansions: accurate both near the mean as well as in the tail regions.