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

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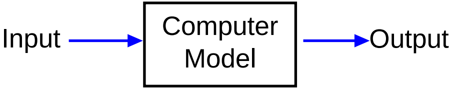
UQ components and methods



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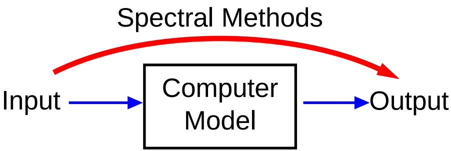
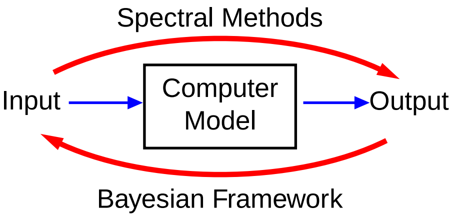


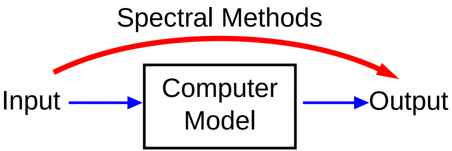
- Sensitivity analysis
  - Small parameter perturbations
- Predictability assessment
  - Larger parameter uncertainties

UQ components and methods



- Sensitivity analysis
  - Small parameter perturbations
- Predictability assessment
  - Larger parameter uncertainties
- Parameter estimation
  - Inverse problems

UQ components and methods



- Forward UQ methods
  - Direct (intrusive)
    - Derive new forward model
    - Intrusive Spectral Projection (ISP)
  - Sampling (non-intrusive)
    - Monte-Carlo, Quasi Monte-Carlo
    - Non-intrusive Spectral Projection (NISP)

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 any random variable as a polynomial of a standard random variable

- 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:
  (continuous) Gauss-Hermite, Legendre-Uniform,
  (discrete) Poisson-Charlier.

[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: $r \approx p_{\boldsymbol{c}}(\lambda) = \sum_{k=0}^{K} c_k P_k(\lambda)$

- Approximation model:

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

- Noise model postulated: $\sigma(\lambda, r)$

- Likelihood function:

$$\log P(\mathcal{D}|\mathcal{M}_{\boldsymbol{c}}) = \sum_{i=1}^{N} \log\left(P(z_i|\mathcal{M}_{\boldsymbol{c}})\right) = -\sum_{i=1}^{N} \frac{\left(z_i - g(\lambda, r)\right)^2}{2\sigma(\lambda, r)^2}.$$

Bayesian Inference of the Location of Discontinuity

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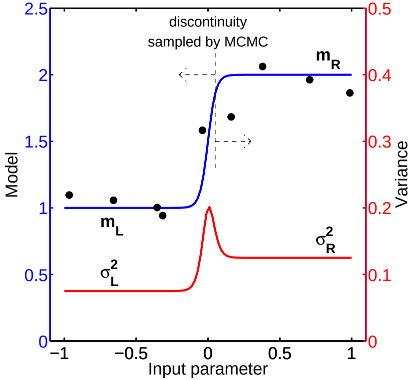
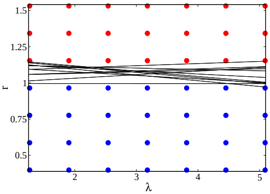
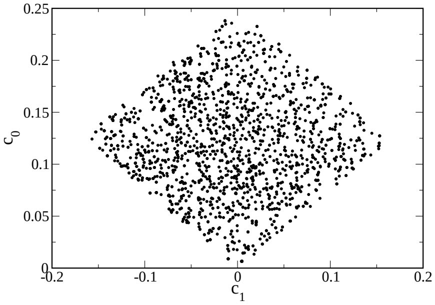
- Bayes' formula: $P(\mathcal{M}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{M})P(\mathcal{M})}{P(\mathcal{D})}$

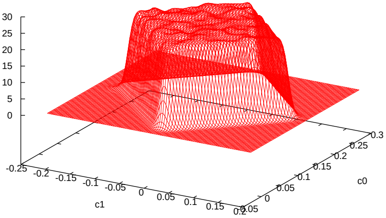


Discontinuity Detection - Highlights

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







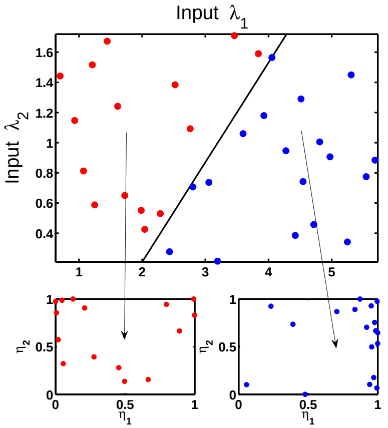
Discontinuity curve samples and their pdf

Parameter Domain Mapping via Rosenblatt Transformation

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

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

- Apply the RT mapping to both sides of the discontinuity



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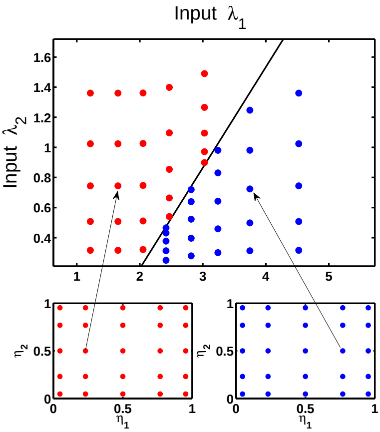

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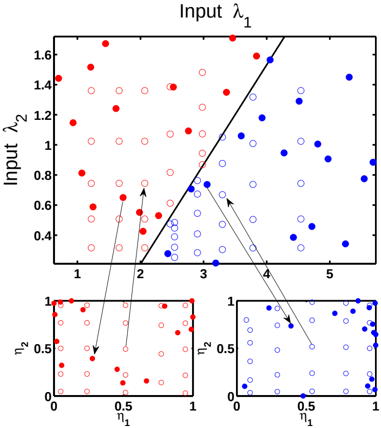

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- Apply the RT mapping to both sides of the discontinuity

PC Expansion, Averaged Over Discontinuity Curves

- PC expansion for each discontinuity curve sample:

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

- Model expansion depends on the parameter location:

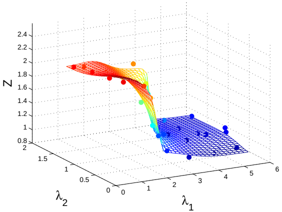
$$Z_{\mathbf{c}}(\vec{\lambda}) = \begin{cases} Z_{\mathbf{c}}^{L}(\vec{\lambda}) & \text{if } (\vec{\lambda}) \in D_L \\ Z_{\mathbf{c}}^{R}(\vec{\lambda}) & \text{if } (\vec{\lambda}) \in D_R \end{cases}.$$

- Average over all PC expansions via RT:

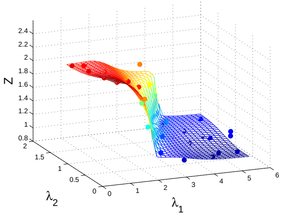
$$\hat{Z}(\vec{\lambda}) = \int_C p(\mathbf{c}) Z_{\mathbf{c}}(\vec{\lambda}) d\mathbf{c} = \int_{[0,1]^{K+1}} Z_{R^{-1}(\vec{\eta})}(\vec{\lambda}) d\vec{\eta}$$

Discontinuous Data Represented Well with the Averaged PC

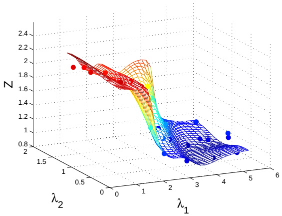
PCE Coefficients via Bayesian Inference



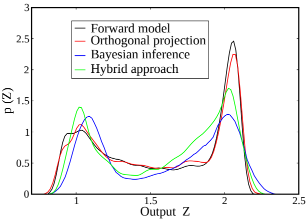
PCE Coefficients via Hybrid Approach



PCE Coefficients via Quadrature Projection



Output PDF



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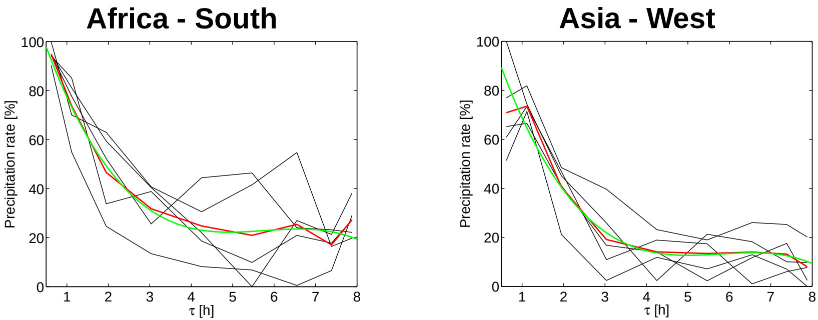
Tackle two of the challenges encountered in forward UQ:

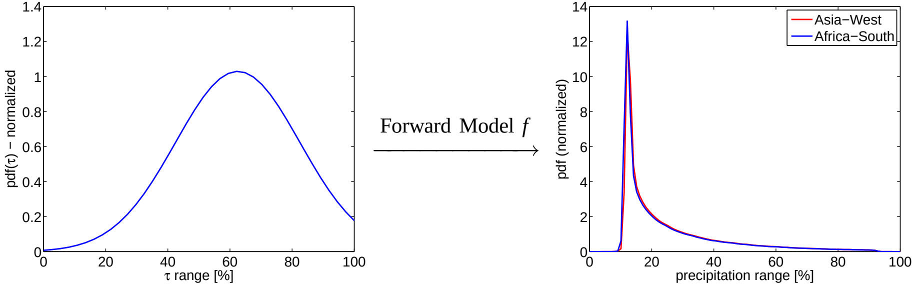
2. Model predictions exhibit fat-tailed distributions.

Precipitation Data from Climate Simulations



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

Forward UQ: Input Parameter PDF → Output Observable PDF



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

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

Polynomial Chaos Expansions and Galerkin Projection

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

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

with

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

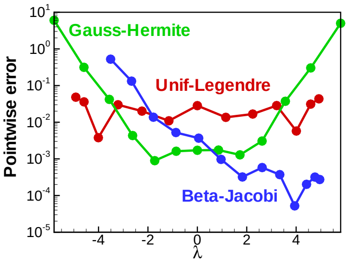
- Galerkin (orthogonal) projection

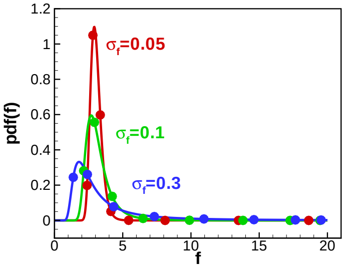
$$Z_k = \frac{\langle f(\lambda(\xi))\Psi_k(\xi)\rangle}{\langle \Psi_k^2(\xi)\rangle}$$

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

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

Non-conventional and Custom Basis Functions

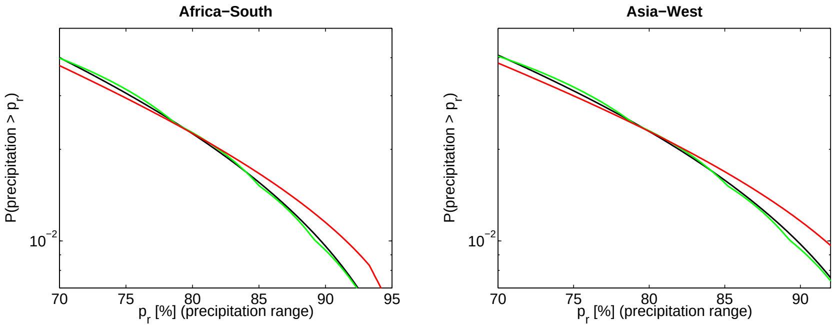




- LU : independent of position
- GH : worse in “tails”, away from the origin
- JB : small in desired region, i.e. it is controllable!

- Design custom polynomials that are orthogonal with respect to fat tailed distributions to get a better accuracy in the tail region.
- 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 climate 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.