Uncertainty Quantification in Climate Modeling

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Uncertainties in Climate Modeling

- Uncertainty sources
  - Parameter uncertainty
    - Model parameters
    - Initial/boundary conditions
    - Model geometry/structure
  - Model/structural uncertainty
    - Unknown physics
    - Reduced order models
  - Scenario uncertainty
    - Policy restrictions
    - Technology improvement
  - Intrinsic variability
    - Stochastic physics
  - Numerical errors

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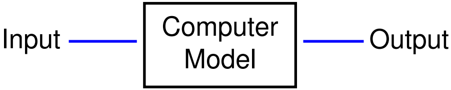
- Need UQ for...
  - Model validation
  - Confidence assessment
  - Optimal design
  - Data assimilation

UQ components and methods



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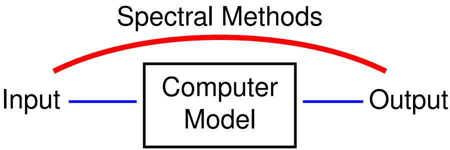

- Sensitivity analysis
  - Small parameter perturbations
- Predictability assessment
  - Larger parameter uncertainties

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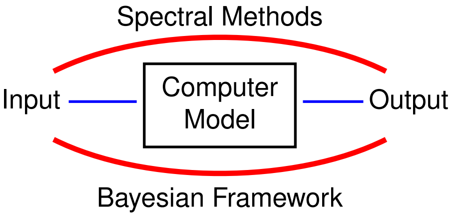
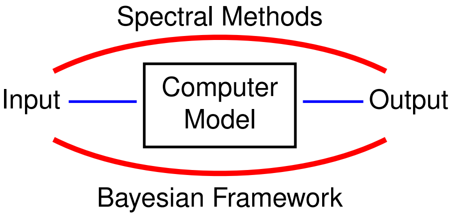


- Sensitivity analysis
  - Small parameter perturbations
- Predictability assessment
  - Larger parameter uncertainties
- Parameter estimation/calibration
  - Inverse problems

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)

Non-Intrusive Spectral Projection (NISP)

- Polynomial Chaos expansions for input γ and output Z

$$\gamma \approx \sum_k \gamma_k \Psi_k(\xi)$$

$$Z = f(\gamma) \approx \sum_k f_k \Psi_k(\xi)$$

- Orthogonal projection via quadrature to obtain PC modes

$$f_k = \int f(\gamma)\Psi_k(\xi)\mathrm{pdf}(\xi)d\xi \approx \sum_* f(\gamma(\xi^*))w^*$$

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Challenges tackled in more detail today

- non-linearities/bifurcations

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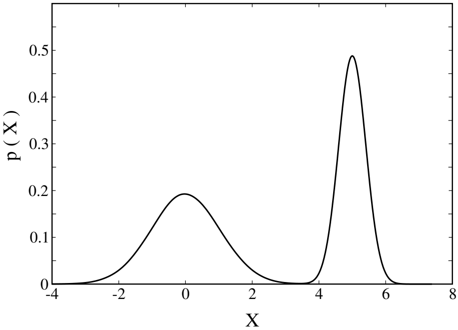
- low-probability/high-impact events

UQ methods are challenged by..

- Nonlinearities, Bifurcations, Bimodalities
- Tail regions
- Limited data
- Intrinsic stochasticity
- Curse of dimensionality



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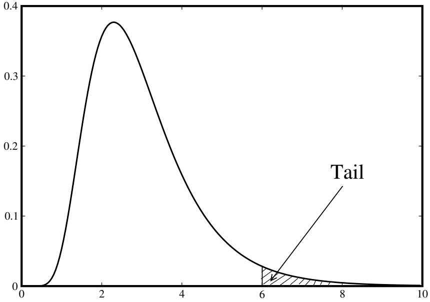

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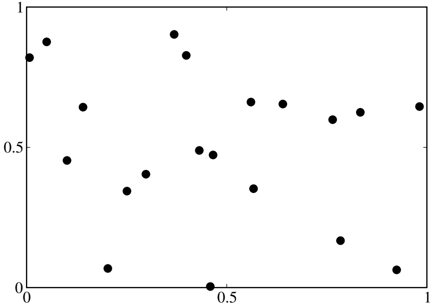

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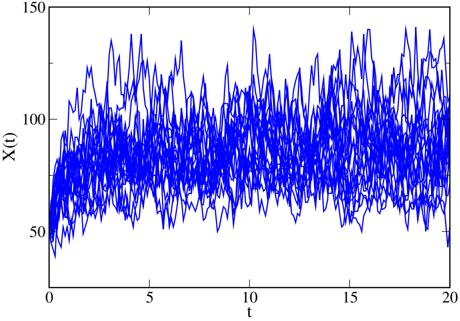

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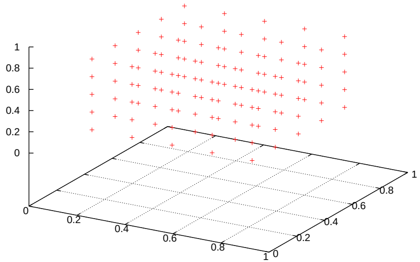

UQ Challenges

- non-linearities/bifurcations
- low-probability/high-impact events
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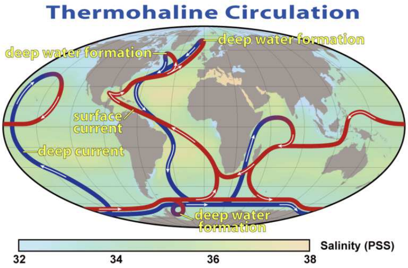
Discontinuities/Nonlinearities/Bifurcations

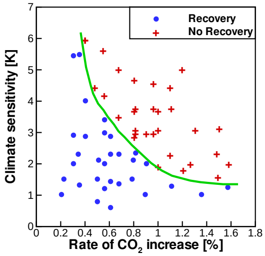
- Stochastic domain decomposition
  - Wiener-Haar Expansions, Multiwavelets [Le Maître *et al*, 2004,2007]
  - Multielement PC [Wan & Karniadakis, 2009]
- Data domain decomposition [Sargsyan *et al*, 2009,2010]
  - Data clustering
  - Mixture PC expansions

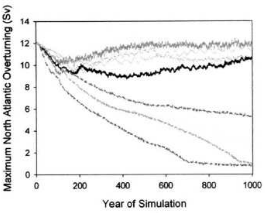
- Adaptive setting
- Does not scale with dimensionality
- For expensive models, can not split much
- *Need a 'smart' domain decomposition*

Webster et al - J. Environ. Syst. 31: 39-59, 2007

- Computational model - EMIC
- Input parameters
  - Rate of CO_2 increase (r)
  - Climate sensitivity (λ)
- Output observable
  - Overturning streamfunction (Z)







Global representations fail to capture discontinuities

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- Input parameters
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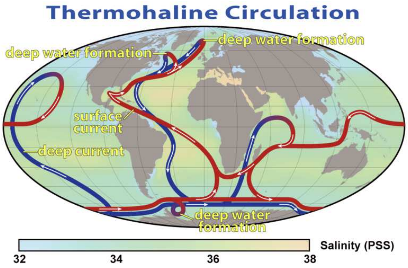
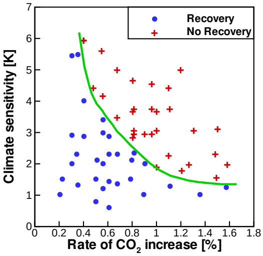
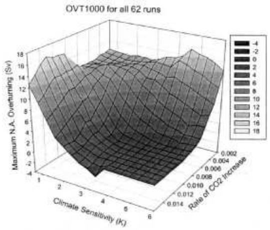






UQ & Discontinuities - Proposed Methodology

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.

Two-step approach:

- **Bayesian inference of the location of the discontinuity**
- **Polynomial chaos representation via parameter domain mapping at each side of the discontinuity**

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:

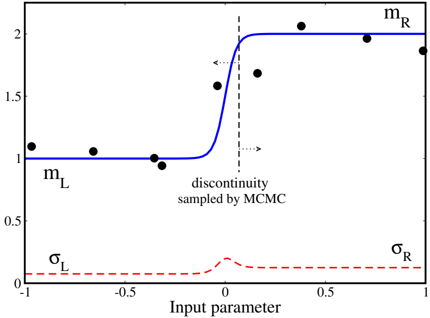
$$\mathcal{M}_{\boldsymbol{c}} \equiv g(\lambda, r) = m_L + (m_R - m_L)\frac{1 + \tanh\left(\alpha(r - p_{\boldsymbol{c}}(\lambda))\right)}{2}$$

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

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

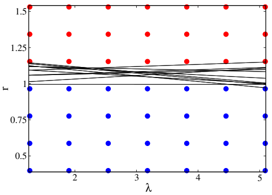
Bayesian Inference of the Location of Discontinuity

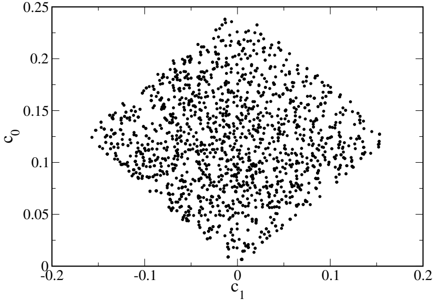
- Parameterize the discontinuity: $r \approx p_{\mathbf{c}}(\lambda) = \sum_{k=0}^{K} c_k P_k(\lambda)$
- Bayes' formula: $P(\mathcal{M}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{M})P(\mathcal{M})}{P(\mathcal{D})}$

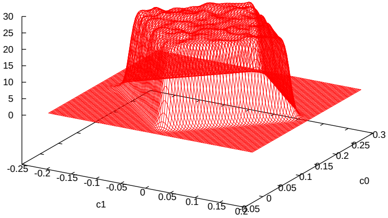


Highlights

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







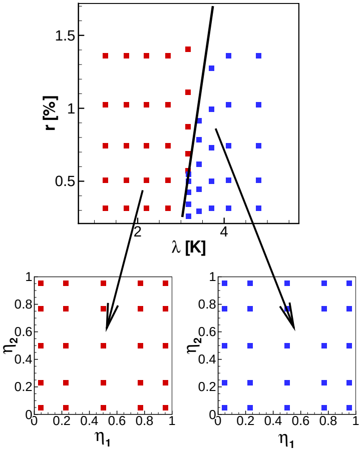
Discontinuity curve samples and their pdf

Parameter Domain Mapping

- 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:

$$\lambda = F_{\lambda}^{-1}(\eta_1),$$
$$r = F_{r|\lambda}^{-1}(\eta_2|\eta_1)$$

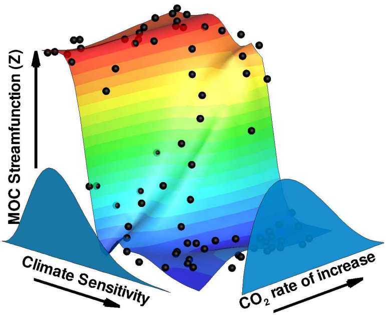
- Apply the RT mapping to both sides of the discontinuity



ROSENBLATT TRANSFORMATION: $(\lambda, r) \rightarrow (\eta_1, \eta_2)$

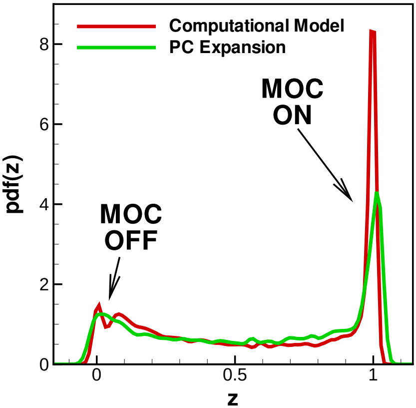
Discontinuous data represented well with the averaged PC

PCE IN (η_1, η_2) DOMAIN



Discontinuous data represented well with the averaged PC.

OUTPUT PDF



Resulting output PDF given input parameter joint PDF.

Summary

- A methodology for uncertainty quantification in climate models with limited data and discontinuities was proposed:
  - Bayesian approach to detect and parameterize the discontinuity as well as the uncertainty associated with it.
  - Rosenblatt transformation maps each of the irregular domains to rectangular ones where the application of the local spectral methods of uncertainty propagation is feasible.
- “Knowledge Discovery from Climate Data: Prediction, Extremes, and Impacts” Workshop Proceedings - 9th IEEE International Conference on Data Mining, 2009.
- Full paper in preparation.

UQ Challenges

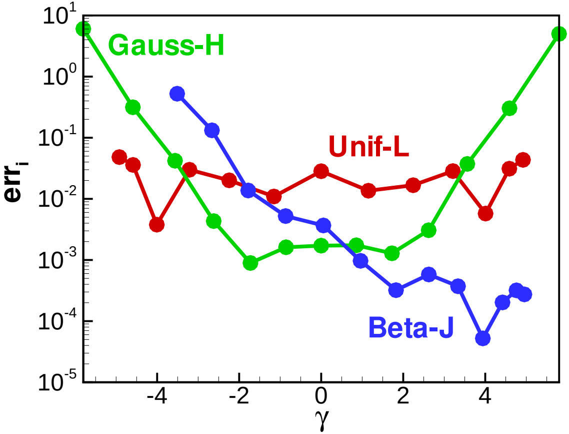
- non-linearities/bifurcations
- low-probability/high-impact events
- limited data
- intrinsic stochasticity
- high dimensionality

Dealing with 'fat' tails

- Several climate observables (e.g. climate sensitivity) exhibit heavy tails
  - require a significant number of simulations to obtain a good sampling of these regions
- Construct spectral expansions based on...
  - Non-classical bases that cluster points in the tail region
  - Bases tailored to the expected behavior of the output
- Use spectral expansions for...
  - Propagating distributions from input parameters to output observables
  - Surrogate models to accelerate the inference process in inverse problems

Pointwise error is large at low-probability regions

$$Z = f(\gamma) \approx \sum_k f_k \Psi_k(\xi) \Longrightarrow f_k = \int f(\gamma)\Psi_k(\xi)\mathrm{pdf}(\xi)d\xi \approx \sum_* f(\gamma(\xi^*))w^*$$



Non-classical quadrature points span the tails better

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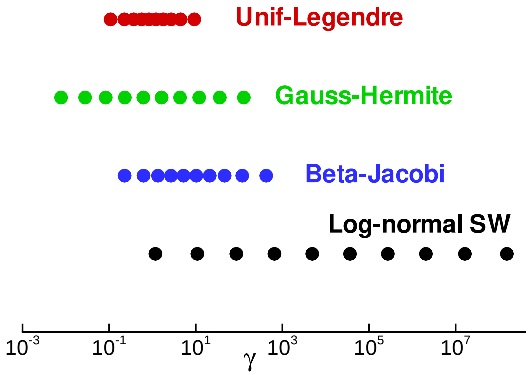

Build a custom PC based on input distribution

- Classical PCEs for input γ and output Z
  - ξ is normal, $\Psi_k(\cdot)$ are Hermite - standard!

$$\gamma \approx \sum_k \gamma_k \Psi_k(\xi)$$

$$Z = f(\gamma) \approx \sum_k f_k \Psi_k(\xi)$$

- *Customized* PCE for output Z with respect to input distribution:
  - γ is *any*, $\Phi_k(\cdot)$ are found by orthogonalization.

$$\gamma = \gamma \qquad \text{(as 'optimal' as it gets)}$$

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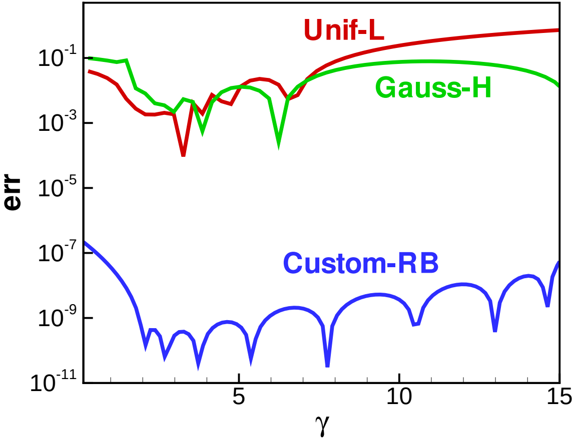
Custom PC Expansions show much better convergence than standard PCE

Input γ belongs to Roe-Baker climate sensitivity distribution.
Synthetic forward model: $f(\gamma) = \cos(\gamma)$



Switching gear...

UQ Challenges

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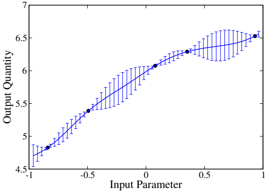
Limited Data

Both observational experiments and computer model simulations are expensive.

- Need to infer functional representation based on limited number of model runs/experiments.
  - Interpolation (kriging)
  - Gaussian Process emulation to assess the lack-of-knowledge [O'Hagan]
  - Extended to stochastic model setting



- *Bayesian* experimental design
  - What are the best locations to take observations?
  - At which parameter sets to run climate models to gain maximal information?

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Intrinsic stochasticity

- Stochastic computer models
- Probabilistic representation of the lack-of-knowledge
- *Climate buzzword:* Stochastic Physics [Palmer & Williams, 2009]

- See previous talk
  (Bert Debusschere on Stochastic Reaction Networks)
- Extend Gaussian Process emulation of deterministic codes to the stochastic case

be Bayesian!!

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Curse of Dimensionality

- (Dimension-adaptive) Sparse quadrature integration
- High Dimensional Model Representation (HDMR)
  - would not handle discontinuities
  - 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]

short answer: no free lunch

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Summary

- Nonlinearities, Bifurcations, Bimodalities
  - Probabilistic detection of discontinuities followed by domain mapping and polynomial chaos expansions to construct model "surrogates".
- Tail regions
  - Employ spectral basis that cluster quadrature points in the tail to construct surrogate models.
  - Construct custom spectral basis based on "expected" shape of the climate model output to improve convergence of the spectral expansion.

Current and future work

- Bring in real climate model data
- Still prohibitively many model runs required: possibly give up orthogonal projection in favor of Bayesian inference
- Experimental design: inform climate modelers on the optimal parameter sets to run simulations
- Gaussian process emulation
  - Couple with PC, either
    a) PC as the mean trend, or
    b) uncertain integration via Bayes-Hermite quadrature.
- Patching PC expansions: capture both the mean and the tail regions

- Climate Science for a Sustainable Energy Future (CSSEF)
  - Multi-lab, multi-year project
  - UQ needed for calibration, validation and prediction

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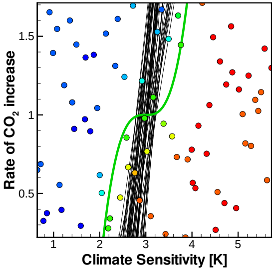
Inference of Discontinuity - 3^{rd} order polynomial

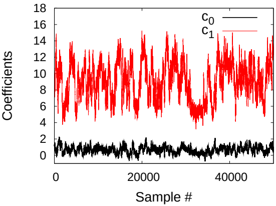
- Synthetic discontinuous data

$$z_i = (1 + \sigma\xi)\,\mathrm{erf}\left(\beta(r_i - \tilde{r}(\lambda_i))\right).$$

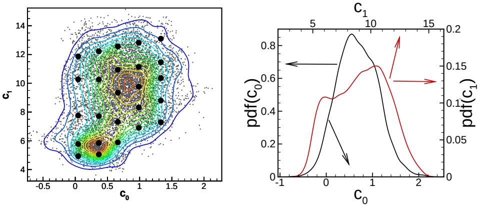
- Use straight lines to infer the discontinuity

$$\tilde{r}(\lambda) = c_0 + c_1\lambda.$$





MCMC samples



Joint and Marginal Posterior Distributions

PC expansion, averaged over discontinuity curves

- PC expansion for each discontinuity curve sample:

$$Z_{\boldsymbol{c}}^{L,R}(\lambda, r) = \tilde{Z}_{\boldsymbol{c}}(\eta_1, \eta_2) = \sum_{p=0}^{P} z_p \Psi_p^{(2)}(\eta_1, \eta_2)$$

- Model expansion depends on the parameter location:

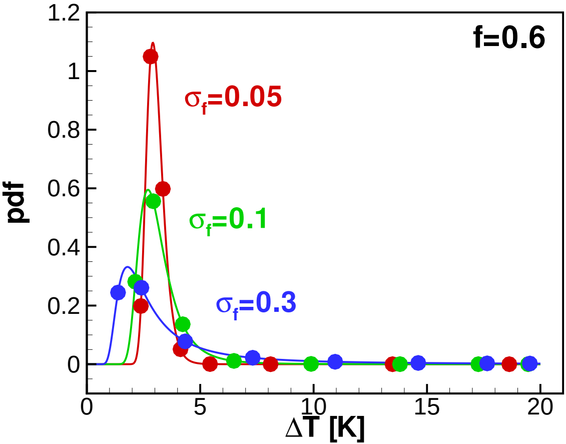
$$Z_{\boldsymbol{c}}(\lambda, r) = \begin{cases} Z_{\boldsymbol{c}}^{L}(\lambda, r) & \text{if } (\lambda, r) \in D_L \\ Z_{\boldsymbol{c}}^{R}(\lambda, r) & \text{if } (\lambda, r) \in D_R \end{cases}.$$

- Average over all PC expansions via RT:

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

Custom Basis' Quad Points Extend to the Tail

(pdf shape from Roe & Baker, Science 2007)



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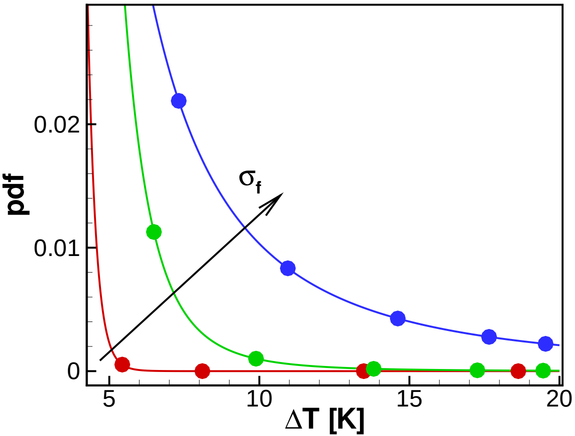
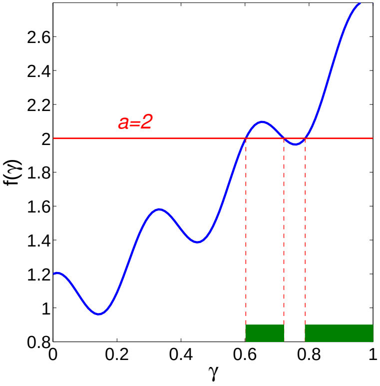


Accuracy of tail probabilities

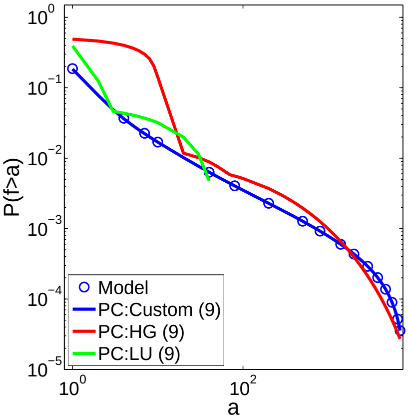
$$P(f > a) = \int_{\gamma:f(\gamma)>a} \mathrm{pdf}(\gamma)d\gamma$$

- Compare $P(f_{exact} > a)$ against $P(f_{PC} > a)$.
- Accuracy depends both on
  - $|f_{exact} - f_{PC}|$.
  - how accurate are the the regions where $f > a$.



Test probability errors

- Forward model:
  $f(\gamma) = \exp(0.5\gamma - 1)$
  - γ is a truncated log-normal
- PC expansions:
  - Legendre polynomials
  - Hermite polynomials
  - Custom basis (truncated log-normal)



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