RAVEN Workshop

Advanced UQ With Collocation Methods

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Overview

Overview: Session Goal

Use advanced methods to accelerate UQ

- For low dimensionality, far fewer runs
- For smooth respones, provides accurate ROMs
- ROMs contain analytic mean, variance, sensitivities

Motivations

Motivations: Monte Carlo

Gold standard in UQ is Monte Carlo, Latin Hypercube

- Consistently convergent (central limit theorem)
- Easy to develop
- Error diminishes slowly
- Requires $1/\epsilon^2$ samples to achieve error ϵ

Motivations: Alternatives to Monte Carlo

Some structured samplers can improve greatly on Monte Carlo
Example: Stochastic Collocation for generalized Polynomial Chaos

- Expand model in orthogonal polynomials
- Use integration to determine expansion coefficients
- Quadrature methods perform polynomial integrations

Input dimensions need to be orthogonalized before running

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Methods

Methods: generalized Polynomial Chaos expansion

$$f(x) \approx G(x) = \sum_{k \in \Lambda} c_k \Phi_k(x), \tag{1}$$

where

- $f(x)$ is the original model,
- x are the uncertain inputs in $f(x)$,
- $G(x)$ is the generalized Polynomial Chaos expansion,
- k is a multi-index to a polynomial, e.g. (3,1,2),
- Λ is a pre-determined set of polynomial indices,
- c_k are expansion coefficients,
- $\Phi_k(x)$ are multidimensional orthogonal polynomials

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Methods: gPC Coefficients

$$f(x) \approx G(x) = \sum_{k \in \Lambda} c_k \Phi_k(x), \tag{2}$$

$\Phi_k(x)$ are orthogonal,

$$c_k = \int_{\Omega} \rho(x) f(x) \Phi_k(x) dx \tag{3}$$

where $\rho(x)$ is the joint probability distribution.
Numerically, use quadratures for c_k

$$c_k \approx \sum_{\ell=1}^{L} w_\ell f(x_\ell) \Phi_k(x_\ell)) \tag{4}$$

where w_ℓ are the weights and x_ℓ are the points

Methods: Large Dimensionality

Tensor SCgPC only efficient if $N < 4$
Fight curse of dimensionality using Sparse Grids

- Hyperbolic Cross
- Total Degree
- Smolyak Quadrature

Methods: SCgPC in RAVEN

TODO add code: ROM, Sampler, RomTrainer, MultiRun

Methods: Interpolation Node

What if I want to use a different quadrature? What if some dimensions require higher-order polynomials than others?
Specify through an interpolation node TODO example

Methods: Adaptive

What if I don't know what dimensions are higher order?
Use the Adaptive SCgPC sampler! TODO code

Methods: Sobol Decomposition

Methods: Sobol Decomposition

Another kind of expansion

$$\begin{aligned} f(x,y,z) =& f_0 \\ & + f_1(x) + f_2(y) + f_3(z) \\ & + f_{1,2}(x,y) + f_{1,3}(x,z) + f_{2,3}(y,z) \\ & + f_{1,2,3}(x,y,z), \end{aligned}$$

where $f_1(x) = \int\int f(x,y,z)\,dy\,dz$, etc.
Benefits:

- Many problems dominated by low-order interacations
- Provides easy access to Sobol sensitivities
- Each sub-term can be modelled as SCgPC ROM
  - Most are dimension 2 or less!
- Can also be constructed adaptively
  - Highest efficiency: Adaptive Sobol with Adaptive SCgPC

Demonstration: Attenuation Problem

Reminder: the Model

$$f(x) = \prod_{n=1}^{N} \exp(-x_n/N), \tag{5}$$

$$x_n \sim \mathcal{U}(0,1). \tag{6}$$

Taylor expansion suggests many combinations of high-order terms

$$\exp(-x) = 1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \cdots \tag{7}$$

Expected:

- Tensor Product, Total Degree, Adaptive perform well
- Hyperbolic Cross should struggle