Adaptive Sparse-Grid Stochastic Collocation Uncertainty Quantification

A Ph.D. Research Proposal

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February 23, 2015

1 Motivation

- With the increase of numerical models, UQ is critical.
- For low-dimension uncertainty space, MC is inefficient.
- Generalized polynomial chaos (gPC) is a suitable surrogate approximation.
- Stochastic collocation (SC) is very efficient compared to MC for small input spaces.
- Sobol decomposition is a natural extension of gPC.

2 Theory

2.1 gPC

- Represent stochastic process as sum of product of weighted sets of orthonormal polynomials
- Index Sets determine combination of polynomial orders to use based on truncation level L
- Further, use anisotropy to increase polynomial focus where sensitivity is highest

2.2 SC

- To determine coefficients for polynomial products, use quadrature integration
- Use Smoljak-like sparse grids to alleviate curse of dimensionality

2.3 HDMR/Sobol decomposition

- First decompose QoI into reference, singlet, duplet, etc. terms
- Second, evaluate each sub-term using SC for gPC
- Doesn't improve on gPC generally for convergence, but provides sensitivities
- For large dimension, can use nested quadrature to reduce work necessary

3 Demonstrated Results

3.1 Static Sparse Grid

3.1.1 Analytical Function, $N = 5$

- TD best, HC next, MC last (5 inputs)
- Exponential convergence for TD

3.2 Projectile, $N = 8$

- HC best, TD next, MC last
- Demonstrate lower regularity

3.3 Reactor Core

- $N = 5$
  - HC best, TD next, MC last
  - Similar convergence between index sets
- $N = 14$
  - On-par with Monte Carlo

3.4 Anisotropic Sparse Grid

- Correctly chosen, always improves convergence
- Incorrectly chosen, slower convergence
- Can unexpectedly increase total computations for the same polynomial level L for large anisotropy (compared to isotropic sparse grid)

3.5 Sobol Decomposition (HDMR)

- Sparse grid accomplishes nearly the same effect as HDMR
- However, HDMR still good for sensitivity analysis and creating anisotropic weights

4 Intended Research

4.1 Adaptivity

- Polynomial selection - add polynomial choices in any dimension/combination of dimensions until contribution is less than a relative tolerance.
  - Algorithm:
  - Loop: start with minimal index set, e.g. $\{(0,0,0),(1,0,0),(0,1,0),(0,0,1)\}$, calculate SC for gPC variance
  - In each dimension, and each combination of dimensions that are only 1 greater than each existing dimension order, add a point
  - See the contribution from each point to the new variance, and close off any dimensions that are converged to tolerance
  - Continue until all dimensions/combinations of dimensions are converged
  - Using a database of nested points, few additional evaluations should be needed each iteration.
- HDMR - Similarly, choose component Sobol factors to be included, then solve each one using adaptive SC for gPC.
  - Algorithm:
  - Outer loop: add terms in HDMR
  - Inner loop: create surrogate model for each term using AASC for gPC
  - If new term contributes less than tolerance, consider dimensions varied to be converged.
  - Stop adding terms in a dimension if all the lower-order terms for the dimension are converged.
  - Continue until all dimensions and combinations are converged.

4.2 Surrogate Modeling

- Feature of interest: limit search algorithm - This particular existing `RAVEN` tool adaptively chooses points to solve in order to define a limiting surface, e.g. between "success" and "failure" regions. Failure probability is integral of failure region.
- Computationally expensive to directly solve algorithm each sample, so use gPC as surrogate model instead
- Metric for Adaptive Anisotropic Sparse Grid Stochastic Collocation for Generalized Polynomial Chaos expansion: ability to determine limit surface and failure probability accurately.
- Suggested problem: irradiated fuel in cladding, power ramp up until fuel touches cladding, do limit search around limiting Von Mises stress.