An Overview of Select UQ Algorithms and their Utility in Applications

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Sparse Quadrature in PC UQ

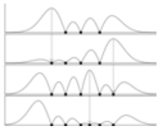
Relevance

- Non-intrusive, sampling-based, UQ methods have general utility
  - Black box handling of computational codes
  - Independent embarrassingly parallel runs
- Polynomial Chaos (PC) non-intrusive Galerkin methods
  - Quadrature-based numerical evaluation of projection integrals
  - Each quadrature point is a computational sample
- High-dimensional setting (e.g. large # uncertain inputs)
  - Care is required to minimize # requisite samples

⇨ Efficient sparse quadrature methods

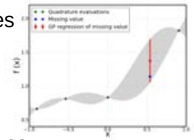
Adaptive Sparse Quadrature and Collocation

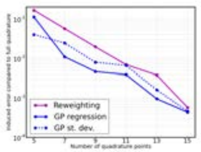
- Avoid dense tensor product grid sampling
- Target sparse optimal set of points
- Use Leja sequences to greedily generate 1D points that are approximately optimal for weighted interpolation
  - Non-isotropic, Adaptive



Fault-Tolerant Quadrature

- Quadrature relies on availability of all samples
- Investigate alternative integration methods with missing quadrature evaluations
  - Quadrature reweighting
  - Polynomial regression
  - Gaussian process estimate of missing values
- Missing a single quadrature point reduces the quadrature formula accuracy (polynomial exactness) by a factor of two.

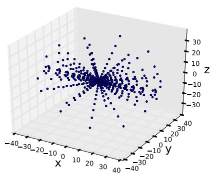




GP regression estimates the missing values with a similar accuracy as re-weighting, but also provides error-bars on the final answer

Evaluation of quantum chemistry integrals

- Developing sparse quadrature techniques for integration arising in 2nd-order many-body perturbation theory (MP2)
- Enhancing sparse quadrature with spherical transformations
- BES partnership initiated with UIUC



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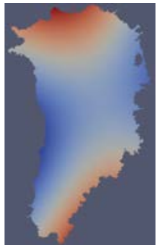
Random Fields

Relevance

- Many applications involve uncertain inputs/outputs that have spatial or time dependence
- Such an uncertain function, represented probabilistically, is a random field/process.
  - It is a random variable at each space/time location
  - Generally with some correlation structure in space/time
  - An infinite-dimensional object
- The Karhunen Loeve expansion (KLE) provides an optimal representation of random fields, employing a (small) number of eigenmodes of its covariance function

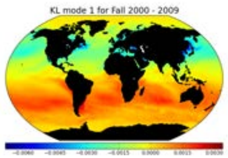
Ice Sheet Basal Boundary Layer

- We wish to quantify uncertainty in predictions of sea level rise from ice-sheet melting.
- Friction between an ice sheet and the land mass is the first order uncertainty effecting predictions of sea level rise.
- The friction is a random field which can be represented using a KLE.
- Current study involves inferring friction B*(x,y)* from field measurements of surface velocities
- BER PISCEES partnership with UT



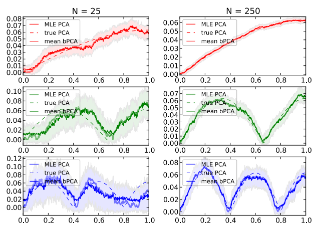
Sea Surface Temperature

- We perform a KLE/PCA analysis of NOAA's sea surface temperature data for the past three decades.
- The figure to the right shows the magnitude of the first KL mode for the Fall months from 2000 – 2009.
- This data set has ~10^6 dimensions



Bayesian PCA

- Uncertain KLE given limited # of samples; Bayesian framework
- Compute principal directions of maximum variance
- Produce error bounds on the principal modes themselves
- The figure shows PCA modes in solid colored lines overlaid with the uncertainty: shaded regions.



More samples, less uncertainty

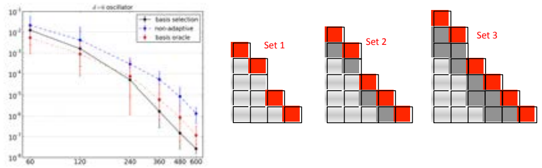
Compressed Sensing

Relevance

- Many physical models have a large # of uncertain inputs
- UQ in this high-dimensional setting is a major computational challenge – too many samples and/or large # PC modes
- Yet physical models typically exhibit sparsity
  - A small number of inputs are important
- Seek sparse PC representation on input space
  - Small number of dominant terms
- Compressed sensing (CS) is useful for discovering sparsity in high dimensional models
- Identify terms that contribute most to model output variation
- Ideal for when data is limited

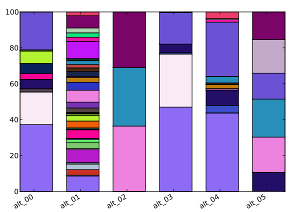
Basis selection

- Cardinality of total degree basis grows factorially with the number of uncertain inputs.
- Even for lower dimensional problems redundant basis terms can degrade accuracy
- To reduce redundancy and improve accuracy the PCE truncation can be chosen adaptively.



Sparsity in Atmospheric Modeling

- QOI : time averaged profile of ozone concentration
- 95 dimensional input space
- Adaptive: start with first order terms, successively adding higher order terms
- 2nd-order approximation
  - 25-150 terms
  - Full 2nd-order: ~4500 terms
- BER ACES4GCM partnership



Sensitivity indices for ozone at six different altitudes. Each color represents a different input parameter: reactants *e.g.* CO