Adaptive approximations of computationally intensive models for uncertainty propagation and inference

Patrick R. Conrad and Youseff M. Marzouk

Introduction
- Practical problems in uncertainty propagation, sensitivity analysis, and inference require using computationally expensive forward models, e.g., $f(x)$
- Standard algorithms require an intractable number of evaluations
- Constructing surrogate $\tilde{f}(x)$ can lower the overall cost of the analysis

Part 1: Forward uncertainty propagation
- Polynomial chaos expansions (PCEs) are used to approximate functions of known random variables:
  $$\tilde{f}(x) = \sum_x (\Psi(x))$$
- $\Psi$ are orthonormal polynomials; $f$ are Fourier coefficients
- Customizable to various domains and measures
- Extends to higher dimensions via tensor products
- Adaptive Smolyak algorithms allow a flexible and practical construction
- Well-suited to uncertainty propagation

Pseudospectral approximation in one dimension
- We can analytically compute coefficients:
  $$f(x) = \sum_{i=0}^{\infty} f_i \psi_i(x) = \sum_{i=0}^{\infty} (f(x), \psi_i(x)) \psi_i(x)$$
- Pseudospectral approximations use quadrature to compute the integral
  $$\mathcal{S}_i[f(x)] = \sum_{i=0}^{\infty} \mathcal{Q}_i[(f(x)), \psi_i(x)]$$
- Choose truncation and quadrature so that every $\psi_i^2$ is integrated correctly

Smolyak algorithms
- Smolyak approach builds sparse tensor product algorithms from one-dimensional algorithms; good for problems with weak input coupling
- Let
  $$\Delta^0_i = \epsilon^0_i = 0$$
- Form the telescoping sum
  $$L^0 = \sum_{k=i}^{\infty} \Delta^0_i$$
- Smolyak’s algorithm is
  $$A(m, d, L) = \sum_{k=i}^{\infty} \Delta_i^0 \cdots \Delta_k^{d-1} L_k$$
- or:
  $$A(K, d, L) = \sum_{k=i}^{\infty} \Delta_i^0 \cdots \Delta_k^{d-1} L_k$$

Termination criteria
- The global error indicator is typically well-correlated with $L^0$ error, except for non-smooth functions
- Samples might be allocated as shown, drawn with density similar to the posterior density
- These samples may be used to construct local linear or quadratic approximations

Adaptivity
- Smolyak algorithms are more efficient only if the index set is suited to the problem at hand
- Add indices incrementally, based on empirical local error indicator
  $$\epsilon_k := \| \Delta^0_k \cdots \Delta^d_k \|_2$$
- where $\Delta^0_k \cdots \Delta^d_k$ is a PCE and $\| \cdot \|_2$ is a $L^0$ norm over the input space
- Halt adaptation with a global error indicator
  $$\epsilon_g := \sum \epsilon_k$$

Example of adaptivity
- A fabricated example in an exponential growth Gaussian quadrature setting

Combustion model example
- Model computes the ignition time of a methane/air mixture, based on 14 uncertain input rate parameters
- Testing adaptive and non-adaptive strategies with different growth rules

Adaptive local approximations
- When performing inference, it is difficult to efficiently choose distributions for input parameters to build a PCE
- This example shows how the samples are largely drawn from regions of low posterior mass
- Instead, we aim to build an approximation that is accurate over the posterior

Part 2: Inference and inverse problems

Adaptive and inverse problems
- On each iteration, when Markov chain Monte Carlo needs to evaluate the approximate forward model, construct/update the approximation as follows

Algorithm outline
- Construct best surrogate using only $S_N$
- Estimate $\psi(x)$
- Optimize over $R$ using penalized $\epsilon(x)$
- Run $f(x^*)$, select $x^*$
- Accept/reject $x^*$
- Return $\Omega_{x^*}(x^*)$

Genetic toggle switch
- Infer six parameters of a kinetic model simulating a genetic toggle switch
- Test performance by performing inference repeatedly, with or without approximations

Conclusions
- Uncertainty quantification tasks can be made tractable with surrogates
- Adaptive polynomial approximations are well-suited to uncertainty propagation
- Novel surrogates can exploit the structure of inference problems

Support from the SciDAC program funded by the US Department of Energy, Office of Science, Advanced Scientific Computing Research under award number DE-SC0007099; part of the SciDAC QUEST Institute (Quantification of Uncertainty in Extreme Scale Computations).
Contact: preconrad@mit.edu, ymarzouk@mit.edu