UQTk
A Flexible Python/C++ Toolkit for Uncertainty Quantification

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## Acknowledgements

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1. General Characteristics
2. Surrogate Construction
3. Bayesian Model Inference and Comparison
4. Summary
5. References
UQ is about enabling predictive simulations

Experiments

Predictive Simulation

\[ \frac{\partial}{\partial t} (\theta \rho \tilde{Y}_i) + \nabla \cdot (\theta \rho \tilde{Y}_i \tilde{u}) = \nabla \cdot (\theta \tilde{S}_i) + \theta \tilde{\omega}_i + \tilde{\omega}_{si} \]

Theory
UQ methods extract information from all sources to enable predictive simulation

- UQ not just about propagating uncertainties
- The term UQ covers a wide range of methods
An example UQTk workflow

- **Model** $f(\lambda)$
- **Surrogate** $fc(\lambda)$
- **Data** $D = \{y_i\}$
- **Likelihood** $D$
- **Prior** $p(\lambda)$
- **Posterior** $p(\lambda|D)$
- **Prediction** $p(g(\lambda)|D)$
- **Any model** $g(\lambda)$

- **Forward UQ**
- **Inverse UQ**
UQTk provides tools to build a general UQ workflow

- Tools for
  - Representation of random variables and stochastic processes
  - Forward uncertainty propagation
  - Inverse problems
  - Sensitivity analysis
  - Dimensionality reduction
  - Bayesian Compressive Sensing
  - Low Rank Tensors
  - Gaussian Processes
  - ...

- Tools can be used stand-alone or combined into a general workflow
UQTk is meant to be straightforward to download, install and use

- **Target usage:**
  - Rapid prototyping of UQ workflows
  - Algorithmic research in UQ
  - Tutorials / educational
  - Expertise in UQ methods (or a desire to acquire it) helpful

- **Released under the GNU Lesser General Public License**
  - Current version 3.0.4
  - Version 3.1.0 planned for later this year

- No massive third party libraries to download, install, and configure
UQTk is used in a variety of applications

- Direct collaborations
  - US DOE SciDAC FASTMath institute
    https://fastmath-scidac.llnl.gov/
  - Variety of US DOE SciDAC partnership projects
  - Part of US DOE BER E3SM climate model analysis tools
- Many other research groups at universities, National Labs, and industry
- Always welcome new applications / collaborations
- Mailing lists
  - uqtk-announce@software.sandia.gov
  - uqtk-users@software.sandia.gov
• ≈ 900 total downloads
• ≈ 200 downloads of version 3.x
We rely on Polynomial Chaos expansions (PCEs) to represent uncertainty

- Standard PC Basis types supported:
  - Gauss – Hermite
  - Uniform – Legendre
  - Gamma – Laguerre
  - Beta – Jacobi

- Also support for custom orthogonal polynomials
  - Defined by user-provided three-term recurrence formula

- Both intrusive and non-intrusive PC tools provided
  - Primarily Galerkin projection methods
  - Some regression approaches offered through Bayesian Compressed Sensing module

- See also Debusschere, *et al.* 2004; Sargsyan, *et al.* 2014
UQTk uses a combination of C++ and Python

- Main libraries in C++
  - PCBasis and PCSet classes: PC tools (intrusive and non-intrusive)
  - Quad class: quadrature rules (full tensor and sparse tensor product rules)
  - MCMC, Gproc, ...

- Functionality available via
  - Direct linking of C++ code
  - Standalone apps
  - Python interface based on Swig (UQTk version 3.0)

- Download as tar file and configure with CMake
- Examples of common workflows provided
Upcoming Features in UQTk 3.1.0

- **New Functionality**
  - Canonical Low Rank Tensor (LRT) Representations
  - Data Free Inference (DFI) Library
  - tempered MCMC (tMCMC)

- **Enhanced functionality**
  - Python scripts for model evidence computation
  - Python class for Bayesian Compressed sensing
  - Additional examples and tutorials

- **Expected Fall 2018**
  - Sign up for the announcement mailing list
  - uqtk-announce@software.sandia.gov
Longer Term Plans

- Coupling with other libraries
  - Better support for user specified third-party libraries, e.g. random number generators, integrators, ...
  - Coupling with DAKOTA and MUQ for leveraging functionality
- Mixed PC basis types
- More general multi-index specification
- Data structures amenable to parallelization and GPU acceleration
- Other developments you would like to see?
  - Let us know at uqtk-users@software.sandia.gov
Outline

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Bayesian Compressed Sensing

- $N$ training data points $(x_n, u_n)$ and $K$ basis terms $\psi_k(\cdot)$
- Projection matrix $P^{N \times K}$ with $P_{nk} = \psi_k(x_n)$
- Find regression weights $c = (c_0, \ldots, c_{K-1})$ so that

$$u \approx Pc$$

or

$$u_n \approx \sum_k c_k \psi_k(x_n)$$

- The number of polynomial basis terms grows fast; a $p$-th order, $d$-dimensional basis has a total of $K = (p + d)! / (p!d!)$ terms.
- For limited data and large basis set ($N < K$) this is a sparse signal recovery problem $\Rightarrow$ need some regularization/constraints.

- Least-squares

$$\arg \min_c \left\{ \| u - Pc \|_2^2 \right\}$$

- The ‘sparsest’

$$\arg \min_c \left\{ \| u - Pc \|_2^2 + \alpha \| c \|_0 \right\}$$

- Compressive sensing

$$\arg \min_c \left\{ \| u - Pc \|_2^2 + \alpha \| c \|_1 \right\}$$
Bayesian Compressed Sensing

- \( N \) training data points \((x_n, u_n)\) and \( K \) basis terms \( \psi_k(\cdot) \)
- Projection matrix \( P^{N \times K} \) with \( P_{nk} = \psi_k(x_n) \)
- Find regression weights \( c = (c_0, \ldots, c_{K-1}) \) so that

\[
\begin{align*}
\mathbf{u} &\approx \mathbf{Pc} \\
\text{or} \quad u_n &\approx \sum_k c_k \psi_k(x_n)
\end{align*}
\]

- The number of polynomial basis terms grows fast; a \( p \)-th order, \( d \)-dimensional basis has a total of \( K = \frac{(p+d)!}{p!d!} \) terms.
- For limited data and large basis set \((N < K)\) this is a sparse signal recovery problem \(\Rightarrow\) need some regularization/constraints.

- Least-squares \( \arg \min_c \{\|u - Pc\|_2^2\} \)
- The ‘sparsest’ \( \arg \min_c \{\|u - Pc\|_2^2 + \alpha \|c\|_0\} \)
- Compressive sensing Bayesian \( \arg \min_c \{\|u - Pc\|_2^2 + \alpha \|c\|_1\} \)
- Likelihood Prior

Debusschere – SNL UQTk
BCS removes unnecessary basis terms

\[ f(x, y) = \cos(x + 4y) \quad \text{and} \quad f(x, y) = \cos(x^2 + 4y) \]

The square \((i, j)\) represents the (log) spectral coefficient for the basis term \(\psi_i(x)\psi_j(y)\).
Iterative BCS: iteratively increase the order for the relevant basis terms while maintaining the dimensionality reduction [Sargsyan et al. 2014], [Jakeman et al. 2015].

Combine basis growth and reweighting!
Low-Rank Approximations

- Univariate function representation: $p + 1$ coefficients

$$u(\xi) = \sum_{k=0}^{P} u_k \psi_k(\xi)$$

- Multivariate function representation: $P + 1 = \frac{(n+p)!}{n!p!}$

$$u(\xi_1, \ldots, \xi_n) = \sum_{k=0}^{P} u_k \prod_{i=1}^{n} \psi_{\alpha_k^i}(\xi_i)$$

- Low-rank approximation: $r \ast (p_1 + p_2 + \ldots + p_n)$

$$u(\xi_1, \ldots, \xi_n) = \sum_{k=1}^{r} w_k^{(1)}(\xi_1) \ldots w_k^{(n)}(\xi_n)$$
Minimization Problem for Coefficients

- Minimization problem:

\[
\min_{\tilde{u} \in \mathcal{M}} \| u(\xi) - \tilde{u}(\xi) \|^2 + \lambda \mathcal{R}(\tilde{u}(\xi))
\]

where \(\mathcal{M}\) is a suitable tensor subset (Canonical, Tensor Train) and \(\mathcal{R}\) is a regularization function.

- Selection of optimal rank \(r\) and regularization coefficient \(\lambda\) using cross validation.

- Pros: Linear increase in parameters with dimension.

- Cons: Non-linear optimization problem. Optimal approximation \(\tilde{u}(\xi)\) is often not known.
Low Rank Tensor and Bayesian Compressed Sensing Applied to Gauss Genz Function

\[ u(x) = \exp \left( - \sum_{i=1}^{d} w_i^2 (x_i - b)^2 \right), \ w_i = 1, \ b = 0.5 \]

- Box plot over 21 replica tests
- Low-rank approach performs well on function with inherent low-rank structure
Low Rank Tensor and Bayesian Compressed Sensing Applied to Gauss Genz Function

- \( u(x) = \exp \left( - \sum_{i=1}^{d} w_i^2 (x_i - b)^2 \right) \), \( w_i = \frac{1}{i^3} \), \( b = 0.5 \)
- Box plot over 21 replica tests
- Bayesian compressive sensing does well on function with inherent sparsity and low number of samples
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Bayesian Inference and Model Comparison

- Model for thermodynamic properties of RedOx active materials
- Used in design of materials for solar thermochemical Hydrogen production
- General model form $\delta = f(p_{O_2}, T)$
  - Model A: 4 parameters
  - Model B: 8 parameters
- Bayesian parameter inference and model comparison
- Joint work with Dr. Ellen Stechel at Arizona State University
- Funded by the DOE Office of Energy Efficiency and Renewable Energy (EERE)
Bayesian Inference and Model Comparison

- Employed UQTk Python Bayesian Inference tools to infer parameters and compare the two models.
- Model properties and numerical settings specified via flexible xml input file.
- Python postprocessing and model evidence computation.
- Workflow will be part of UQTk 3.1.0 release later this year.
Both models agree well with data

- Model A (left) and Model B (right)
Both models agree well with data

- Model B (right) has smaller residuals
Posterior distributions were sampled with adaptive MCMC

- Well-defined uni-modal distributions
- Model B has more dependencies between its parameters
Model evidence favors model B

- Model evidence computed from posterior samples, using a Gaussian approximation
  - Model A: $\ln(\text{evidence}) = 1580$
  - Model B: $\ln(\text{evidence}) = 1939$
- Despite its higher complexity, model B is clearly favored.
- For situations with more measurement noise, or fewer data points, a simpler model maybe preferred
Summary

- UQTk provides a powerful set of tools for building general UQ workflows
- Multiple ways to access functionality
  - Direct linking of C++ code
  - Standalone apps
  - Python interface based on Swig
- Available at http://www.sandia.gov/UQToolkit
- Suggestions for improvements welcome!
- Do not hesitate to contact us uqtk-users@software.sandia.gov
References

- UQ Tutorials: http://www.quest-scidac.org/outreach/tutorials/