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Some Comments on the Future of Uncertainty Quantification Research

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Broad and Increasing Interest in UQ

- Continuing increase in interest in UQ
  - internationally
  - across disciplines
- Why?
  - Customers:
    - Promise of improved understanding of models/predictions
    - Model validation
    - Making sense of conflicting data/models
  - Practitioners:
    - Range of applied math and statistics challenges
    - Theory, Modeling, algorithms, and software challenges
    - Interesting multidisciplinary work across:
      - applied math, statistics, information theory, data science
    - Availability of funding!

Interesting UQ Research Directions – 1

- Dimensionality reduction
  - Sparse regression, smoothness, low-rank tensor methods
  - Basis adaptation, active subspace
  - Model reduction, low dimensional manifolds
  - Data/Likelihood-informed subspaces
- Sampling for forward UQ and surrogates
  - Adaptive sparse quadrature, optimal regression, QMC, etc
  - Computational strategies for neighbor samples – borrow strength
  - Adaptive surrogate constructions
- Mesh error
  - Probabislitic numerics
  - Mesh error modeling
  - Multilevel methods
- Model complexity
  - Model error in hierarchical models
  - Multifidelity methods
  - Inference on models, model selection
  - Likelihoods with chaotic dynamics

Interesting UQ Research Directions – 2

"Data Science" and statistics

- Machine learning – logistic regression
- Significant advances made over past decade involve
  - Convolutional neural networks
  - Deep neural networks
  - Large training data sizes

  Result in training that learns not only best-fit NN weights but also best-choice of features of the data for high prediction success rate

Opportunities for UQ – ML two-way coupling

- UQ $\Rightarrow$ ML :
  - Bayesian training of neural network models – posterior on weights
  - Bayesian model selection on network models
  - Bayesian classification with NNs
- ML $\Rightarrow$ UQ :
  - Stochastic optimization strategies used in NN training, useful for UQ
  - Data+model-based methods for low-D manifold discovery
  - Identify features in model dynamics that control emergent behavior
  - Correlation vs causality analysis

Interesting UQ Research Directions – 3

Optimization under uncertainty

- Derivative free optimization
  - Black box models
  - Noisy objectives/constraints aside from uncertainty
    - Smooth/well-behaved integral QoIs from deterministic simulations can be noisy due to finite-sized spatiotemporal averages
- MLMF strategies
- Rare event estimation

Stochastic Galerkin – Intrusive methods

- Governing equations – well-posedness, physical constraints
- Numerical methods – stability, convergence, consistency
- Automatic code generation – similar to automatic differentiation