Final Report: Large-Scale Optimization for Bayesian Inference in Complex Systems

Project duration:
15 Aug 2008 – 14 Aug 2013 (for grant number DE-FG02-08ER25858)
15 Sep 2009–14 Sep 2013 (for grant number DE-SC0002517)

Final report submitted by Massachusetts Institute of Technology (MIT)

M Frangos, J Li, C Lieberman, Y Marzouk, K Willcox

1 Project Overview

The SAGUARO (Scalable Algorithms for Groundwater Uncertainty Analysis and Robust Optimization) Project focused on the development of scalable numerical algorithms for large-scale Bayesian inversion in complex systems that capitalize on advances in large-scale simulation-based optimization and inversion methods. The project was a collaborative effort among MIT, the University of Texas at Austin, Georgia Institute of Technology, and Sandia National Laboratories. The research was directed in three complementary areas: efficient approximations of the Hessian operator, reductions in complexity of forward simulations via stochastic spectral approximations and model reduction, and employing large-scale optimization concepts to accelerate sampling.

The MIT–Sandia component of the SAGUARO Project addressed the intractability of conventional sampling methods for large-scale statistical inverse problems by devising reduced-order models that are faithful to the full-order model over a wide range of parameter values; sampling then employs the reduced model rather than the full model, resulting in very large computational savings. Results indicate little effect on the computed posterior distribution. On the other hand, in the Texas–Georgia Tech component of the project, we retain the full-order model, but exploit inverse problem structure (adjoint-based gradients and partial Hessian information of the parameter-to-observation map) to implicitly extract lower dimensional information on the posterior distribution; this greatly speeds up sampling methods, so that fewer sampling points are needed. We can think of these two approaches as "reduce then sample" and "sample then reduce." In fact, these two approaches are complementary, and can be used in conjunction with each other. Moreover, they both exploit deterministic inverse problem structure, in the form of adjoint-based gradient and Hessian information of the underlying parameter-to-observation map, to achieve their speedups.

2 Technical Accomplishments

Reduced-order models for large-scale statistical inverse problems. One MIT component of the SAGUARO Project focused on the role of reduced-order models to accelerate conventional sampling methods for large-scale statistical inverse problems. Our research developed new methodology for performing model reduction in both parameter and state spaces. This permits sampling (using a method such as Markov chain Monte Carlo (MCMC)) to be carried out in a low-dimensional reduced parameter space, and also accelerates the many forward model evaluations required to sample the posterior. The challenge of determining reduced-order models in this setting is to come up with a basis that effectively spans the parameter space of interest, an especially difficult task when the parameter space is of high dimension. We address this challenge by formulating the model reduction task as an optimization problem, which we solve using a heuristic but efficient greedy approach that exploits adjoint-based gradients and Hessian information of the parameter-to-observation map.

Inference for prediction. Another component of the MIT effort was the development of a goal-oriented approach to inference of large-scale systems. Inference of model parameters is often one step in a process ending in predictions that support decision in the form of design or control. Incorporation of end goals into the inference process leads to more efficient goal-oriented algorithms that automatically target the most relevant parameters for prediction. In the linear setting, our approach to goal-oriented inference exploits a compelling connection to balanced truncation model reduction. In balanced truncation one obtains a projection-based reduced model that balances the controllability and observability of the underlying transformed system. In the goal-oriented inference context, we present an approach that leads to a balance between the experiment and prediction observability associated with parameter modes. In the linear case, this approach leads to a form of subspace regularization that is dimensionally optimal in the sense that we infer the fewest number of parameters necessary to accurately estimate the predictions required to meet end goals. The inference-for-prediction method exactly replicates the prediction results of either truncated singular value decomposition, Tikhonov-regularized, or Gaussian statistical inverse problem formulations independent of data; it sacrifices accuracy in parameter estimate for online efficiency. The approach was demonstrated for a contaminant transport problem. This grant also supported the initial work to extend the inference-for-prediction approach to nonlinear systems, with application to a model problem in carbon capture and storage.

Stochastic spectral methods for statistical inverse problems. Another MIT effort focused on stochastic spectral methods, which exploit regularity in the dependence of the forward model—both its internal state and outputs—on uncertain parameters. These methods can be applied intrusively (e.g., in a Galerkin formulation) or non-intrusively (e.g., via collocation); the former requires a reformulation of the governing equations, while the latter requires only deterministic forward simulations at a sparse set of quadrature points. In either case, using stochastic spectral methods to propagate prior uncertainty through the forward model yields a surrogate posterior density that is extremely inexpensive to evaluate, often orders of magnitude faster than the true posterior. We established new convergence results that tie the L^2 convergence rate of a stochastic spectral forward solution to the convergence rate, in Kullback-Leibler divergence, of the surrogate posterior distribution. These results were demonstrated numerically on problems with smooth and with discontinuous dependence on the inversion parameters, and with unimodal or multi-modal posterior distributions. Additional computational work focused on the inversion of spatially distributed parameters in a prototypical porous media problem; here, dimensionality reduction was achieved through Karhunen-Loève representations of Gaussian process priors. The inverse problem was cast in a hierarchical Bayesian formulation, where we inferred not only the permeability field but regularization parameters—or equivalently, prior hyperparameters—from data.

We also carried out a detailed comparison between non-intrusive stochastic spectral approximations and projection-based reduced models, articulating the relative advantages and disadvantages of each method in the context of a representative source inversion problem. We show that if the number of full model samples available to create the approximate models is small, then the projection-based approach achieves a more accurate solution to the inverse problem. If however a sufficient number of samples can be used for stochastic collocation, the resulting models are several times more efficient to solve than a reduced-order model of comparable accuracy.

Adaptive surrogates for statistical inverse problems. A final MIT effort focused on the adaptive construction of *posterior-focused* surrogates for Bayesian inverse problems. The construction of globally accurate approximations for nonlinear forward models can be computationally prohibitive and in fact unnecessary, as the posterior distribution typically concentrates on a small fraction of the support of the prior distribution. We developed new approach that uses stochastic optimization—in particular, the cross-entropy method—to construct polynomial approximations over a sequence of measures adaptively determined from the data, eventually concentrating on the posterior distribution. Numerical demonstrations of the adaptive approach on inference problems involving partial differential equations show order-of-magnitude increases in computational efficiency (as measured by the number of forward solves) and accuracy (as measured by posterior moments and information divergence from the exact posterior) over prior-based surrogates employing comparable approximation schemes.

3 Personnel Supported

MIT (Willcox): 1 graduate student, 1 postdoc
MIT/Sandia (Marzouk): 1 technical staff (Aug–Dec 2008; PI Marzouk moved to MIT in Jan 2009), 1 postdoc

4 Publications, Talks, Awards

Publications

1. C Lieberman, "Parameter and State Model Reduction for Bayesian Statistical Inverse Problems," SM Thesis, MIT, February 2009.

2. C Lieberman, K Willcox, O Ghattas, "Parameter and state model reduction for large-scale statistical inverse problems," *SIAM Journal on Scientific Computing*, Vol. 32, No. 5, pp. 2523-2542, August 2010.

3. Y Marzouk, D. Xiu, "A stochastic collocation approach to Bayesian inference in inverse problems," *Communications in Computational Physics*, Vol. 6, pp. 826–847, 2009.

4. Y Marzouk, H Najm, "Dimensionality reduction and polynomial chaos acceleration of Bayesian inference in inverse problems," *Journal of Computational Physics*, Vol. 228, pp. 1862–1902, 2009.

5. *Computational Methods for Large-Scale Inverse Problems and Quantification of Uncertainty*, L. Biegler, G. Biros, O. Ghattas, M. Heinkenschloss, D. Keyes, B. Mallick, Y. Marzouk, L. Tenorio, B. van Bloemen Waanders, K. Willcox (Eds.), Wiley Series in Computational Statistics, January 2011.

6. M. Frangos, Y. Marzouk, K. Willcox, B. van Bloemen Waanders, "Surrogate and reduced-order modeling: a comparison of approaches for large-scale statistical inverse problems," in *Computational Methods for Large-Scale Inverse Problems and Quantification of Uncertainty*, Biegler et al. (Eds.), Wiley Series in Computational Statistics, January 2011.

7. C. Lieberman, K. Fidkowski, K. Willcox, B. van Bloemen Waanders, "Hessian-based model reduction: Large-scale inversion and prediction," *International Journal of Numerical Methods in Fluids* Vol. X, No. Y, pp. xx–xx, 2012.

8. Goal-Oriented Inference: Approach, Linear Theory, and Application to Advection Diffusion. C. Lieberman and K. Willcox, *SIAM Review*, 55-3, 493–519, 2013. Also *SIAM Journal on Scientific Computing*, Vol. 34, Np. 4, pp. 1880–1904, 2012.

9. Goal-oriented inference: Theoretical foundations and application to carbon capture and storage. C. Lieberman, Ph.D. Thesis, Aeronautics and Astronautics, Massachusetts Institute of Technology, June 2013.
10. J. Li, Y. Marzouk. "Adaptive construction of surrogates for the Bayesian solution of inverse problems." Submitted to *SIAM Journal on Scientific Computing*, 2013. arXiv:1309.5524.

Talks

1. Y Marzouk, "Uncertainty and Bayesian inference in inverse problems," ASC Verification & Uncertainty Quantification seminar series, Lawrence Livermore National Laboratory, Livermore, CA, September 2008.
2. K Willcox, "Uncertainty Quantification and Optimization of Complex Systems: The Challenge and Promise of Model Reduction," Applied Mathematics Principal Investigators Meeting, Argonne National Laboratory, Argonne, IL, October 2008.
3. K Willcox, "Model Reduction for Design, Control and Probabilistic Analysis of Large-Scale Systems," Norwegian University of Science and Technology, Trondheim, Norway, October 2008.
4. C Lieberman, "Reduced-order modeling for statistical inverse problems in groundwater flows," New Zealand Institute for Mathematics and its Applications, Programme in Energy, Wind and Water: Algorithms for Simulation, Optimization and Control, Auckland, New Zealand, February, 2009.
5. C Lieberman, "Model Reduction for Uncertainty Quantification in Large-scale Inverse Problems," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
6. Y Marzouk, "Stochastic collocation and Galerkin methods for Bayesian inverse problems," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
7. Y Marzouk, "Nonparametric Bayesian density estimation in hierarchical engineered systems," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
8. K Willcox, "Model Reduction for Uncertainty Quantification and Decision-Making Under Uncertainty," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
9. Y Marzouk, "Uncertainty Quantification and Statistical Inference in Computational Engineering," RWTH-Aachen, Institute for Advanced Study in Computational Engineering Science (AICES), Aachen, Germany, March 2009.
10. K Willcox, "Model Reduction for Uncertainty Quantification in Large-Scale Complex Systems," Seminar Series in Verification, UQ and Sensitivity Analysis, Lawrence Livermore National Laboratory, Livermore, CA, May 2009.
11. K Willcox, "Model Reduction for Uncertainty Quantification and Optimization of Large-Scale Systems," Plenary Talk, SIAM Conference on Applied Linear Algebra, Monterey Bay-Seaside, CA, October 2009.

12. K Willcox, “Model Reduction for Uncertainty Quantification and Optimization Under Uncertainty of Complex Systems,” Workshop on Computing with Uncertainty, Institute for Mathematics and its Applications (IMA), Minneapolis, MN, October 2010.

13. Y Marzouk,“Uncertainty and inference in complex physical problems,” Politecnico di Milano, MOX-MIT workshop on ‘Reduction Strategies for the Simulation of Complex Problems. Milan, Italy, January 2011.

14. Y Marzouk, “Uncertainty and experimental design in complex physical systems,” Georgia Tech, College of Computing seminar, Atlanta, GA, January 2011.

15. Y Marzouk, “Uncertainty and experimental design in complex physical systems,” University of Texas at Austin, Institute for Computational Engineering and Sciences (ICES) seminar, Austin, TX, February 2011.

16. M Parno, Y Marzouk, “Multiscale methods for statistical inference in elliptic problems,” SIAM Conference on Computational Science & Engineering, Reno, NV, March 2011.

17. Y Marzouk, “Multiscale and map-based methods for statistical inference in inverse problems,” Workshop on Stochastic Multiscale Methods, Banff International Research Station (BIRS), Banff, Canada, March 2011.

18. K Willcox, “Model Reduction for Design, Optimization, Inverse Problems and Quantification of Uncertainty in Large-scale Systems,” Singapore-Delft Water Alliance, Singapore, March 2011.

19. Y Marzouk, “Low-rank structure in statistical inverse problems.” Applied Inverse Problems 2011 (invited minisymposium). College Station, TX, May 2011.

20. Y Marzouk, “Bayesian inference for inverse problems: foundations and computational methods.” IMA Workshop on Large-scale Inverse Problems and Quantification of Uncertainty (invited tutorial lectures). Minneapolis, MN, June 2011.

21. Y Marzouk, “Bayesian inference and stochastic spectral methods.” Oberwolfach seminar (invited). Mathematisches Forschungsinstitut Oberwolfach, Germany, June 2011.

22. K Willcox, “Surrogate and Multifidelity Modeling for Optimization Under Uncertainty of Large-scale Complex Systems,” Aachen Conference on Computational Engineering Science, Aachen, Germany, July 2011.

23. K Willcox, “Model Reduction for Large-Scale Systems: Efficient Approaches for Problems with High-Dimensional Parameter Spaces,” Peaceman Lecture on Numerical Mathematics, Rice University, Houston, TX, September 2011.

24. K Willcox, “Model Reduction and Surrogate Modeling for Uncertainty Quantification,” Statistical and Applied Mathematical Sciences Institute (SAMSI) 2011-12 Uncertainty Quantification Program Methodology Opening Workshop, Research Triangle Park, NC, September 2011.

25. K Willcox, “Model Reduction for Large-Scale Systems: Efficient Approaches for Problems with High-Dimensional Parameter Spaces,” Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany, October 2011.

26. J Li, "Adaptive construction of surrogates for Bayesian inference." SIAM Conference on Uncertainty Quantification (UQ12) (invited minisymposium). Raleigh, NC, April 2012.

27. K Willcox, "Model reduction for uncertainty quantification of large-scale systems," Plenary talk, SIAM Conference on Uncertainty Quantification, Raleigh, NC, April 2012.

28. Y Marzouk, "Bayesian inference with spectral approximations and optimal maps." University of Colorado at Boulder, Department of Applied Mathematics. Boulder, CO, April 2012.

29. K Willcox, "Multifidelity Modeling for Identification, Prediction and Optimization of Large-Scale Complex Systems," Plenary talk, SIAM Annual Meeting, Minneapolis, MN, July 2012.

30. K Willcox, "Model reduction for uncertainty quantification of large-scale systems," Special AIAA-SIAM Session on Uncertainty Quantification and Management for Complex Systems, AIAA Multidisciplinary Analysis and Optimization Conference, Indianapolis, IN, September 2012.

31. K Willcox, "Model reduction for systems with high-dimensional parameter spaces," Seminar for Applied Mathematics, ETH Zurich, Switerzland, October 2012.

32. K Willcox, "Model Reduction: Exploiting Structure in Large-Scale Complex Systems," Plenary Talk, MathBio4: Scale Symposium, Madison, WI, October 2012.

33. K Willcox, "Model reduction for systems with high-dimensional parameter spaces," Applied and Computational Math Seminar, George Mason University, VA. Also Numerical Analysis Seminar, University of Maryland, November 2012.

34. K. Willcox, "Multifidelity Modeling for Identification, Prediction and Optimization of Large-scale Complex Systems," Information Science and Technology Seminar, Los Alamos National Laboratory, April 2013.

35. Y Marzouk, "Tractable Bayesian inference in inverse problems: forward approximation and dimension reduction," 38th Woudschoten Conference on Numerical Mathematics (keynote lecture). Zeist, The Netherlands, September 2013.

Awards

1. C Lieberman (graduate student, MIT) received second place in the Bavarian Graduate School of Computational Engineering (BGCE) Student Paper Prize for outstanding student work in the field of Computational Science and Engineering, for his paper and presentation titled "Parameter and state model reduction for uncertainty quantification in large-scale statistical inverse problems." Awarded March 2009 at the SIAM Conference on Computational Science and Engineering, Miami, FL.

2. C. Lieberman and K. Willcox received a SIGEST Award from SIAM for their paper "Goal-Oriented Inference: Approach, Linear Theory, and Application to Advection Diffusion."