Optimization in the Context of Data Assimilation: II

Parameter Estimation and Model Validation in Nonlinear Dynamical Networks

Award DOE-SC0002349

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Abstract

Numerical optimization is a vital component of many state-of-the-art techniques for model synchronization, data assimilation and uncertainty quantification. Although a range of algorithms and software exists for general-purpose optimization, new methods must be developed to meet the challenges posed by the huge optimization problems that arise in DOE applications. These problems have features that make them hard to solve using "off-the-shelf" optimization methods. Their constraint derivatives have a very specialized sparsity structure that reflects, in part, the associated dynamical system. Moreover, the use of mesh refinement for the differential equation constraints means that each optimization problem is just one of a *family* of optimization problems, each with a different size, but related sparsity structure. To add to this complexity, the optimization problems become more difficult as the mesh is refined or new data are added. The exploitation of these properties is critical to the efficiency of the optimization process.

Our approach has been to combine the best features of two state-of-the-art optimization methods: interior-point (IP) methods, and sequential quadratic programming (SQP) methods. IP methods are very efficient when solving large "one-off" problems, in large part because the fixed structure of the equations makes it possible to utilize sophisticated software developed by the linear algebra community. Moreover, IP methods can utilize the second derivatives of the problem functions and have a strong theoretical foundation that does not require the subproblem to be solved exactly when the iterates are far from the solution. On the other hand, SQP methods provide a relatively reliable "certificate of infeasibility" when a subproblem is infeasible (which is typical for a problem associated with a coarse mesh or limited data). Also, SQP methods require only one or two outer iterations when started near the solution—a crucial property as the mesh is refined or new data are added.

A new SQP method has been developed that uses a primal-dual generalized augmented Lagrangian *line-search merit function* to obtain a sequence of improving estimates of the solution. This function is a modern primal-dual variant of the augmented Lagrangian proposed by Hestenes and Powell in the early 1970s. A crucial feature of the new method is that the QP subproblems are convex, but formed from the exact second derivatives of the original problem. This is in contrast to methods that use a less accurate quasi-Newton approximation. Additional benefits of this approach include the following.

- Each QP subproblem is regularized, and has a known feasible point.
- New efficient primal- and dual methods are defined for the QP subproblem.
- The method can be implemented using "black-box" linear algebra software, thereby allowing the exploitation of recent advances in software for multicore and GPU-based architectures.

Preliminary numerical experiments involving the synchronization of models associated with nonlinear dynamical systems indicate that the new method is significantly more efficient than our current SQP package `SNOPT`.