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Global Nonlinear Parameter Estimation Using Interval Analysis: Parallel Computing Strategies

Chao-Yang Gau and Mark A. Stadtherr*
Department of Chemical Engineering
University of Notre Dame, Notre Dame, IN 46556

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*author to whom all correspondence should be addressed; Fax: (219) 631-8366; E-mail: markst@nd.edu

1 Introduction

Parameter estimation is a common problem in many areas of process modeling, both in on-line applications such as real time optimization and in off-line applications such as the modeling of reaction kinetics and phase equilibrium. The goal is to determine values of model parameters that provide the best fit to measured data, generally based on some type of least squares or maximum likelihood criterion. In the most general case, this requires the solution of a nonlinear and frequently nonconvex optimization problem.

It is not uncommon for the objective function in nonlinear parameter estimation problems to have multiple local optima. However, the standard methods used to solve these problems are local methods that offer no guarantee that the global optimum, and thus the best set of model parameters, has been found. Thus, there is a need for global optimization in nonlinear parameter estimation. One approach that has been suggested is the use of convex underestimating functions in connection with a branch and bound procedure (Esposito and Floudas, 1998). An alternative approach for global optimization is the use of interval analysis (e.g., Hansen, 1992). In this presentation we demonstrate the use of interval methods for determining a global optimum in nonlinear parameter estimation problems of interest in process engineering, and consider strategies for using parallel computing to reduce the required wall-clock time in this and other global optimization problems.

2 Methodology

As an example, we consider the estimation of parameters in vapor-liquid equilibrium (VLE) models. We have demonstrated previously (Gau and Stadtherr, 1998) that even for simple models, such as the Wilson equation, multiple local optima can occur in parameter estimation, and that for some data sets, published parameter values (Gmehling and Onken, 1977–1990) correspond to a local but not global optimum. For such cases, a simple global optimization procedure based on interval analysis can be used to reliably determine the globally optimal parameter values. The method used involves the use of an interval-Newton technique combined with interval branch and prune. This method provides a mathematical and computational guarantee of global optimality in parameter estimation. For larger scale problems, the use of parallel computing may be desirable in order to reduce wall-clock time requirements.

By implementing an efficient dynamic workload balancing scheme for tree searching, the performance of the sequential interval branch and prune process in the interval-Newton algorithm can be enhanced. This is done on a distributed memory multiprocessing system using an SPMD (single program, multiple data) programming model and employing the

message-passing protocol MPI. The use of recently developed dynamic workload balancing methods, requiring no global data structure, are studied, including dynamic work-stealing techniques (Blumofe and Leiserson, 1994), and diffusive workload balancing (Heirich and Taylor, 1995). The goal is to reduce the ratio of communication to computation, while maintaining an equilibrium workload at all times, and, therefore, to achieve a speed-up close to the number of processors used.

3 Results and Discussion

Three parallel dynamic workload balancing algorithms were developed and implemented on the top of the sequential interval-Newton technique. These are a synchronous work-stealing algorithm (SWS), a synchronous diffusive workload balancing algorithm (SDWB), and an asynchronous diffusive workload balancing algorithm (ADWB). Each algorithm in this sequence maintains the advantages of and then improves on the performance of the previous one. By applying a distributed workload structure locally on each processor, SWS prevents the bottleneck effect existing in centralized workload balancing algorithms, such as that suggested by Schnepper and Stadtherr (1996). The next algorithm, SDLB, then also takes advantage of a diffusive workload transfer scheme to reduce the probability of idle status in each processor. It also restricts communication to neighborhood processors, in contrast to using extensive global communication. This tends to alleviate the network communication overhead, which would increase substantially as the number of processors applied becomes large, and thereby impede scalability. ADLB maintains the key features of the previous two algorithms, and also applies the special nonblocking communication offered by MPI, breaking the network synchronization to overlap communication and computation and further reduce the communication overhead.

As an example, we consider the estimation of the energy parameters in the Wilson equation for liquid-phase activity coefficients from the binary vapor-liquid equilibrium (VLE) data of the water and formic acid system, as examined by Gau and Stadtherr (1998). The regression estimator assigned as the objective function is maximum likelihood with an unknown diagonal covariance matrix. This represents a difficult four-parameter global optimization problem. The problem was solved on a homogeneous multiprocessing system, composed of up to 16 Sun UltraSPARC 140e workstations as processing units, and connected with switched ethernet. As expected, the most significant speedups are obtained when using the asynchronous diffusive workload balancing algorithm (ADWB), which can achieve a consistently high efficiency ($\sim$90–95%), for up to 16 processors. This performance demonstrates the very good scalability of the ADWB approach for large scale problems.

The workload balancing algorithms implemented are general purpose and can be applied to other global optimization problems. To demonstrate this, we consider a liquid phase

stability problem, a global optimization problem solved using interval analysis, as explained by Tessier et al. (1998). In this case, by using the ADWB approach, superlinear speedups were observed, e.g., speedup by a factor of ∼30 when applying 16 processors. Superlinear speedup is possible in this case because of the nature of the interval branch and bound algorithm used, which, when executed in parallel, tends to result in nodes being eliminated sooner than when executed on a single processor. Thus when executed in parallel, there are not only more processors working on the problem, but fewer nodes to be processed.

4 References

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