New Interval Methodologies for Reliable Process Modeling

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Motivation

• In process modeling, chemical engineers frequently need to solve nonlinear equation systems in which the variables are constrained physically within upper and lower bounds; that is, to solve:

\[ f(x) = 0 \]
\[ x^L \leq x \leq x^U \]

• These problems may:
  – Have multiple solutions
  – Have no solution
  – Be difficult to converge to any solution
Motivation (continued)

- There is also frequent interest in globally minimizing a nonlinear function subject to nonlinear equality and/or inequality constraints; that is, to solve (globally):

\[
\min_{x} \phi(x)
\]

subject to

\[
\begin{align*}
  h(x) &= 0 \\
  g(x) &\geq 0 \\
  x^L &\leq x \leq x^U
\end{align*}
\]

- These problems may:
  - Have multiple local minima (in some cases, it may be desirable to find them all)
  - Have no solution (infeasible NLP)
  - Be difficult to converge to any local minima
Motivation (continued)

- *One* approach for dealing with these issues is *interval analysis*.

- Interval analysis can
  - Provide the engineer with tools needed to solve modeling and optimization problems with complete certainty.
  - Provide problem-solving reliability not available when using standard local methods.
  - Deal automatically with rounding error, thus providing both mathematical and computational guarantees.
Motivation (continued)

- We have successfully applied interval Newton/generalized bisection (IN/GB) methods for
  - General process modeling problems (Schnepper and Stadtherr, 1996).
  - Phase stability and equilibrium problems using several different thermodynamic models (Stadtherr et al., 1994; Hua et al., 1996,1998,1999; Xu et al., 1998,1999).
  - Computation of azeotropes (homogeneous, reactive, heterogeneous) of multicomponent mixtures (Maier et al., 1998,1999).
  - Computation of mixture critical points (Stradi et al., 1998)

- However, the IN/GB algorithm applied to date is very basic, and its performance is unacceptable on some problems.
Interval Method Used

- Interval Newton/Generalized Bisection (IN/GB)
  - Given a system of equations to solve, an initial interval (bounds on all variables), and a solution tolerance
  - IN/GB can find (enclose) *with mathematical and computational certainty* either all solutions or determine that no solutions exist. (e.g., Kearfott 1987, 1996; Neumaier 1990).
  - IN/GB can also be extended and employed as a deterministic approach for global optimization problems (e.g., Hansen, 1992).

- A general purpose approach; in general requires no simplifying assumptions or problem reformulations.

- Current implementation based on modifications of routines from INTBIS and INTLIB packages (Kearfott and coworkers)
Interval Method (Cont’d)

Problem: Solve $f(x) = 0$ for all roots in interval $X^{(0)}$.

Basic iteration scheme: For a particular subinterval (box), $X^{(k)}$, perform root inclusion test:

- (Range Test) Compute an interval extension of each function in the system.
  
  - If 0 is not an element of any interval extension, delete the box.
  
  - Otherwise,

- (Interval Newton Test) Compute the image, $N^{(k)}$, of the box by solving the linear interval equation system

\[ F'(X^{(k)})(N^{(k)} - x^{(k)}) = -f(x^{(k)}) \]

- $x^{(k)}$ is some point in the interior of $X^{(k)}$.
- $F'(X^{(k)})$ is an interval extension of the Jacobian of $f(x)$ over the box $X^{(k)}$. 
There was no solution in $X^{(k)}$
Unique solution in $X^{(k)}$
This solution is in $N^{(k)}$
Point Newton method will converge to it
Any solutions in $X^{(k)}$ are in intersection of $X^{(k)}$ and $N^{(k)}$

If intersection is sufficiently small, repeat root inclusion test; otherwise bisect the result of the intersection and apply root inclusion test to each resulting subinterval.
Interval Method (Cont’d)

Some areas for potential algorithm improvement

• Tightening interval extensions of functions and Jacobian elements.

• Use of different tessellation schemes.

• Tighter bounds on the image \( N^{(k)} \) that encloses the solution set of the interval Newton equation.

  – Preconditioning strategies (focus of this presentation).
Solving the Interval Newton (IN) Equation

• Usually done by one iteration of preconditioned Gauss-Seidel scheme:
  
  – Solve

  \[ Y^{(k)} F'(X^{(k)}) (N^{(k)} - x^{(k)}) = -Y^{(k)} f(x^{(k)}) \]

  – The scalar preconditioning matrix \( Y^{(k)} \) is often chosen to be an inverse midpoint preconditioner \( Y^{inv} \): inverse of the midpoint of the interval Jacobian matrix, or inverse of the Jacobian matrix at midpoint of the interval.

• One performance goal: Find smallest possible enclosure \( N \) of the solution set of the IN equation. The preconditioner used can have a strong effect on performance in this regard.

• Preconditioners that are optimal in some sense have been proposed by Kearfott (1990,1996) based on LP strategies
Preconditioning Strategies

• The preconditioner can be \textit{designed} row by row during the Gauss-Seidel process try to achieve desired goals.

• Consider the \textit{i}-th step of Gauss-Seidel and the \textit{i}-th preconditioner row, \( y_i \),

\[
N_i = x_i - \frac{Q_i(y_i)}{D_i(y_i)}
\]

\[
y_i f(x) + \sum_{j=1}^{n} y_i A_j (X_j - x_j)
\]

\[
= x_i - \frac{y_i A_i}{y_i A_i}
\]

then take \( N_i \cap X_i \). (\( A_i \) is the \textit{i}-th column of the \( F'(X) \) matrix.)

• Elements of \( y_i \) can be chosen to try to meet a desired goal.
Preconditioning Strategies

- Practical optimality criteria for preconditioner row $y_i$:
  - Width-optimal preconditioner row: minimize width of $N_i \cap X_i$.
  - Endpoint-optimal preconditioner row: maximize the lower bound of $N_i$ or minimize the upper bound of $N_i$.

- Optimality can be approached by a scheme in which the preconditioner row contains only one nonzero element. This can be called a pivoting preconditioner $Y^P$.

- We use a new hybrid scheme in which one or more of $Y^{INV}$, width-optimal $Y^P$, or endpoint-optimal $Y^P$ are used, depending on the situation, and following heuristic rules.
Numerical Experiments

• Both equation-solving and global optimization problems were selected to illustrate the improvements that can be achieved using the new hybrid preconditioner.

  – Problem 1: Error-in-variables parameter estimation.
  – Problem 2: Phase stability analysis for LLE system.
  – Problem 3: Computation of critical points of mixtures.
  – Problem 4: Computation of heterogeneous azeotropes.

• We compared use of $Y^{INV}$ alone to use of the new hybrid preconditioner on a Sun Ultra 2/1300 workstation.
Results and Discussion

• Problem 1: Error-in-variables parameter estimation
  – Global optimization with 2 parameter variables and 10 state variables.
  – Point evaluations of objective function done at the midpoint of current box used for bounding in objective range test.
  – Use Van Laar equation to model experimental vapor-liquid equilibrium data.
  – Using $Y^{inv}$ alone took $> 4$ CPU days.
  – Using new hybrid preconditioner took 1504 CPU seconds.
Results and Discussion (cont.)

- Problem 2: Phase stability analysis for LLE system
  - Equation-solving problem with 6 independent variables.
  - Use UNIQUAC model to for computing excess Gibbs energy.
  - Using $Y^{inv}$ alone took 50217 CPU seconds
  - Using new hybrid preconditioner took 152 CPU seconds.
Results and Discussion (cont.)

- Problem 3: Computation of critical points of mixtures
  - Equation-solving problem with 6 variables (four component mixture).
  - Use Peng-Robinson equation of state to model both the liquid and gas phases.
  - Using $Y_{inv}$ alone took 2094 CPU seconds.
  - Using new hybrid preconditioner took 658 CPU seconds.
Results and Discussion (cont.)

• Problem 4: Computation of heterogeneous azeotropes
  – Equation-solving problem with 11 variables (3 components).
  – Use NRTL activity coefficient model.
  – Using $Y^{inv}$ alone took $> 1$ CPU days
  – Using new hybrid preconditioner took 270 CPU seconds.
Concluding Remarks

• Use of the new hybrid pivoting preconditioner scheme provides an approach to manipulate the interval Gauss-Seidel process to achieve greater efficiency.

• This has led to large reductions in CPU time for all problems tested, and in some cases, reductions of 2 or more orders of magnitude.

• For difficult problems, the additional work required to construct the preconditioner is easily overcome by a large reduction in the number of intervals that must be processed.

• For more details, please see the Poster 213c in the High Performance Computing Poster Session, Wednesday, 7pm, Khmer Pavilion.

• These slides will be available next week at http://www.nd.edu/~markst/presentations.html
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