LP-Based Approach for Process Modeling Using Interval Methods

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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:

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}$$

$$\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U$$

- These problems may:
  - Have multiple solutions
  - Have no solution
  - Be difficult to converge to any solution

Motivation (Cont'd)

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

$$\min_{\mathbf{x}} \phi(\mathbf{x})$$

subject to

$$\mathbf{h}(\mathbf{x}) = \mathbf{0}$$

$$\mathbf{g}(\mathbf{x}) \geq \mathbf{0}$$

$$\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U$$

- 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 (Cont'd)

- *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.
- However, the primary drawback to this approach is that computational time requirements may become quite high, so that its performance may be unacceptable on some problems.

Interval Methodology

- 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.
  - IN/GB can also be extended and employed as a deterministic approach for global optimization problems.
- A general purpose approach; in general requires no simplifying assumptions or problem reformulations.
- No strong assumptions about functions need to be made.

Interval Methodology (Cont'd)

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

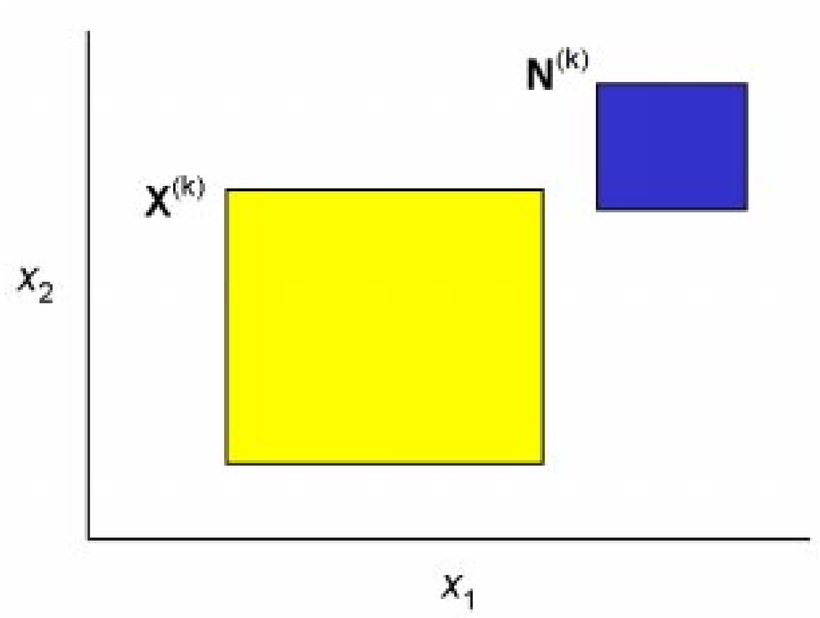
Basic iteration scheme: For a particular subinterval (box), $\mathbf{X}^{(k)}$, perform root inclusion test:

- (Range Test) Compute an interval extension (bounds on range) for 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*, $\mathbf{N}^{(k)}$, of the box by solving the linear interval equation system

$$\mathbf{F}'(\mathbf{X}^{(k)})(\mathbf{N}^{(k)} - \tilde{\mathbf{x}}^{(k)}) = -\mathbf{f}(\tilde{\mathbf{x}}^{(k)})$$

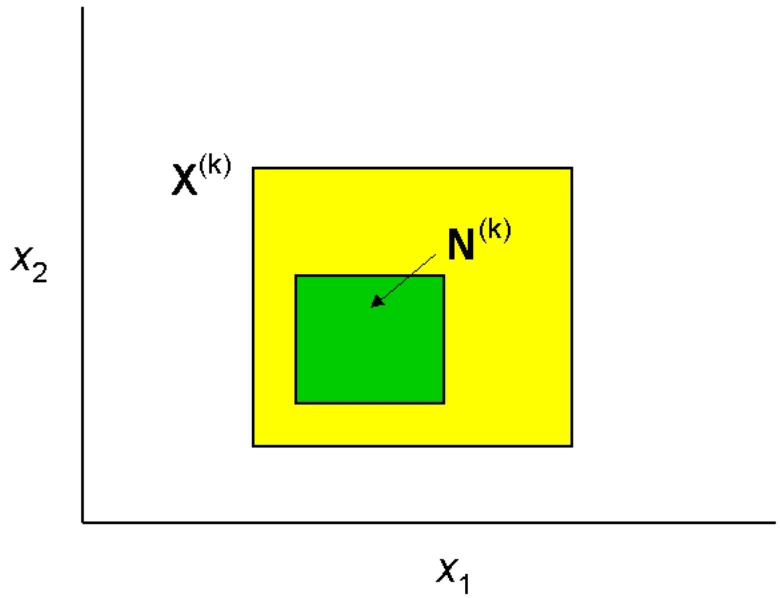
  - $\tilde{\mathbf{x}}^{(k)}$ is some point in $\mathbf{X}^{(k)}$.
  - $\mathbf{F}'\left(\mathbf{X}^{(k)}\right)$ is an interval extension of the Jacobian of $\mathbf{f}(\mathbf{x})$ over the box $\mathbf{X}^{(k)}$.

Interval Methodology (Cont'd)



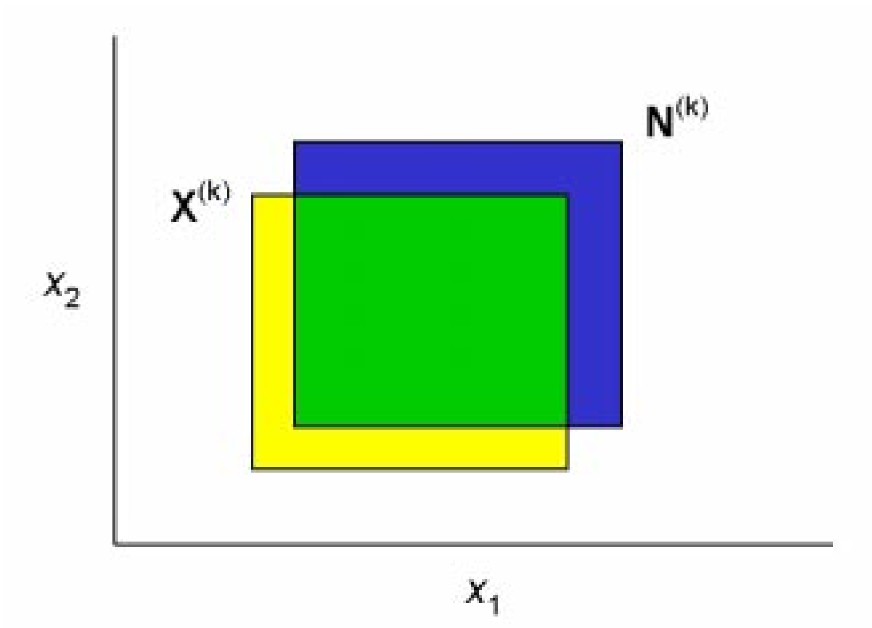
- There is no solution in $\mathbf{X}^{(k)}$

Interval Methodology (Cont'd)



- There is a *unique* solution in $\mathbf{X}^{(k)}$
- This solution is in $\mathbf{N}^{(k)}$
- Additional interval-Newton steps will tightly enclose the solution with quadratic convergence. (Point Newton method will also converge to solution from any point in $\mathbf{N}^{(k)}$.)

Interval Methodology (Cont'd)



- Any solutions in $\mathbf{X}^{(k)}$ are in intersection of $\mathbf{X}^{(k)}$ and $\mathbf{N}^{(k)}$
- If intersection is sufficiently small, repeat root inclusion test
- Otherwise, bisect the intersection and apply root inclusion test to each resulting subinterval

Interval Methodology (Cont'd)

- Can be extended to global optimization problems.
- For unconstrained problems, solve for stationary points.
- For constrained problems, solve for KKT or Fritz-John points.
- Add an additional pruning condition (objective range test):
  - Compute interval extension of objective function.
  - If its lower bound is greater than a known upper bound on the global minimum, prune this subinterval.
- This combines IN/GB with a branch-and-bound scheme.
- Key step, for either optimization or equation solving, is solution of linear interval system

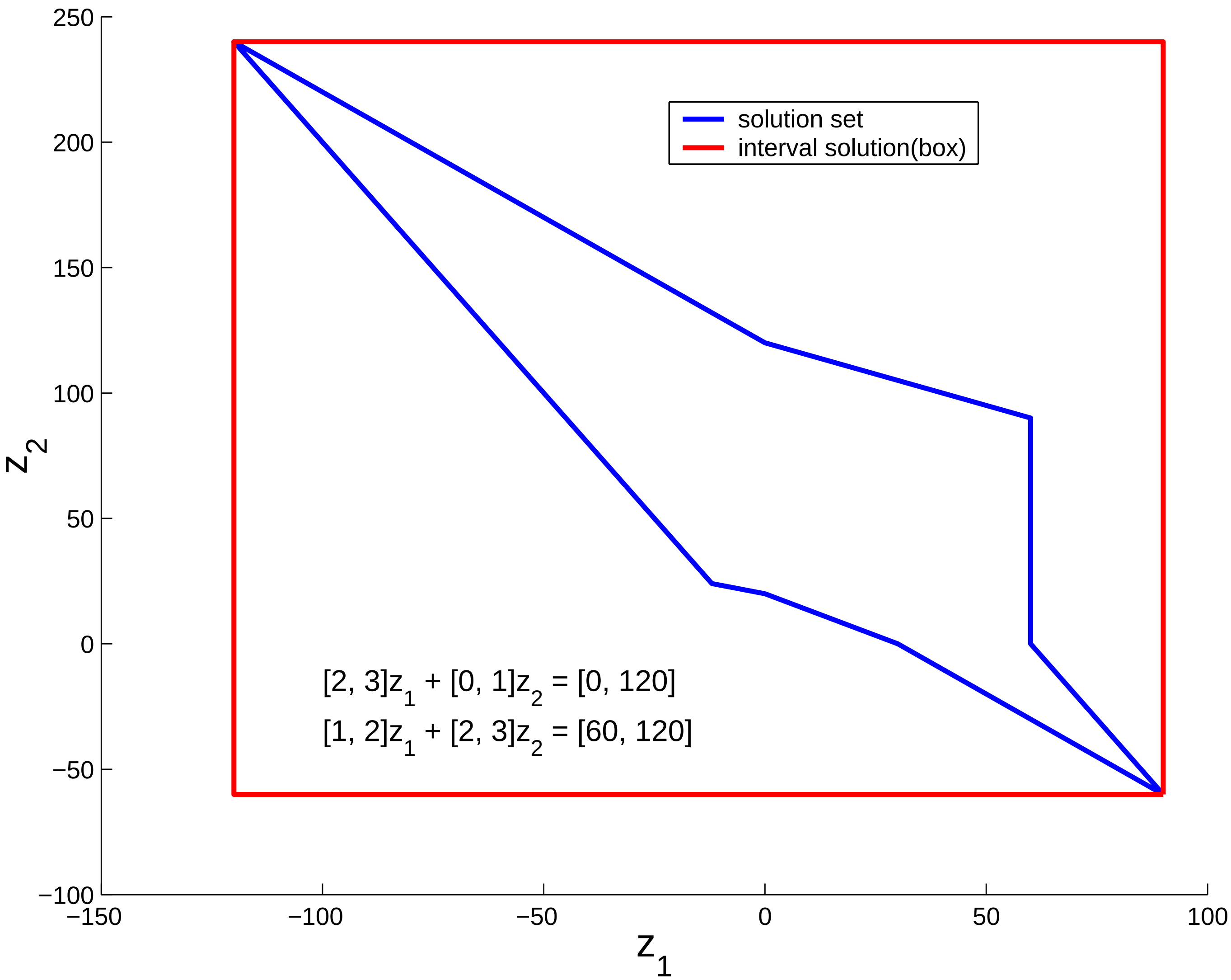
$$\mathbf{F}'(\mathbf{X})(\mathbf{N} - \tilde{\mathbf{x}}) = -\mathbf{f}(\tilde{\mathbf{x}})$$

Seek tightest possible bounds on solution $(\mathbf{N} - \tilde{\mathbf{x}})$, and thus on $\mathbf{N}$.

Solution Set of Linear Interval System

- Consider linear interval system $\mathbf{Az} = \mathbf{B}$.
- Solution set is defined: $\mathbf{S} = \{\mathbf{z} \mid \tilde{\mathbf{A}}\mathbf{z} = \mathbf{b}, \tilde{\mathbf{A}} \in \mathbf{A}, \mathbf{b} \in \mathbf{B}\}$.
- Interval solution: An interval $\mathbf{Z}$ containing $\mathbf{S}$.
- Computing the interval hull (tightest interval containing $\mathbf{S}$) is NP-hard (Rohn and Kreinovich, 1995).
- Several methods are available to compute an interval solution $\mathbf{Z}$ that contains $\mathbf{S}$, but that may not give tight bounds.
- Methods used in the context of interval-Newton:
  - Preconditioned (inverse-midpoint) interval Gauss-Seidel
  - Hybrid (pivoting/inverse-midpoint) preconditioner and real point selection (HP/RP) (Gau and Stadtherr, 2002)
  - **LP strategy**

Solution Set of Linear Interval System



LP Strategy for Linear Interval System

- Oettli & Prager(1964) theorem : Solution set $\mathbf{S}$ is defined by the constraints

$$\left|\hat{\mathbf{A}}\mathbf{z} - \hat{\mathbf{B}}\right| \leq \Delta\mathbf{A}\,|\mathbf{z}| + \Delta\mathbf{B}$$

  $\hat{\mathbf{A}}$ – component-wise midpoint matrix of $\mathbf{A}$

  $\Delta\mathbf{A}$– component-wise half width matrix of $\mathbf{A}$

  $\hat{\mathbf{B}}$ – component-wise midpoint vector of $\mathbf{B}$

  $\Delta\mathbf{B}$ – component-wise half width vector of $\mathbf{B}$

- To eliminate absolute value operation on $\mathbf{z}$, the components of $\mathbf{z}$ must keep a constant sign $\longrightarrow$ consider each orthant separately.

LP Strategy for Linear Interval System (Cont'd)

- In each orthant, define D_α, a diagonal matrix whose entries are α_j:

$$\alpha_j = \begin{cases} 1 & \mathbf{z}_j \geq 0 \\ -1 & \mathbf{z}_j < 0 \end{cases} \quad j = 1, 2, \ldots, n$$

- To determine bounds on $\mathbf{S}$ in each orthant, solve $2n$ linear programming problems:

$$\text{maximize (and minimize)} \quad \mathbf{z}_j, \; j = 1, 2, \ldots, n$$
$$\text{s.t.} \quad \begin{pmatrix} \hat{\mathbf{A}} - \Delta\mathbf{A} D_\alpha \\ -\hat{\mathbf{A}} - \Delta\mathbf{A} D_\alpha \end{pmatrix} \mathbf{z} \leq \begin{pmatrix} \mathbf{B}^U \\ -\mathbf{B}^L \end{pmatrix}$$
$$\alpha_j \mathbf{z}_j \geq 0, \; j = 1, 2, \ldots, n$$

- To get optimal solution overall (interval hull), calculate extrema in all orthants (2^n in worst scenario — exponential complexity)

LP Strategy for Linear Interval System (Cont'd)

Application to IN/GB methods:

- Solve linear interval system

$$\mathbf{F}'(\mathbf{X})(\mathbf{N} - \tilde{\mathbf{x}}) = -\mathbf{f}(\tilde{\mathbf{x}})$$

- Only the part of $\mathbf{N}$ that intersects $\mathbf{X}$ needs to be found.
- If $\tilde{\mathbf{x}}$ is selected to be a corner of $\mathbf{X}$, then the part of $\mathbf{N} - \tilde{\mathbf{x}}$ that lies in $\mathbf{X}$ is entirely in one orthant.
- Solution of interval-Newton equation can be sought using LP in only one orthant. Tightest possible solution obtained, while avoiding exponential time complexity.

Numerical Experiments

- LISS_LP(Linear Interval System Solver by Linear Programming) has been developed.
- Two error-in-variables parameter estimation problems (formulated as unconstrained global optimization) were selected to illustrate the improvements that can be achieved using LISS_LP.
- We compare performance results of LISS_LP to HP/RP (Gau and Stadtherr, 2002) on a SUN Blade 1000 model 1600 workstation.
- Performance results include
  - Number of interval Newton tests performed (I-N tests)
  - CPU time in seconds

Results and Discussion

- Problem 1: Parameter estimation in VLE model (van Laar equation)
- Formulated as unconstrained global optimization with 2 parameter variables and 10 state variables.
- LP solver uses dense linear algebra.

	HP/RP	LISS_LP
I-N tests	303,589	156,182
CPU time (s)	664.4	496.7

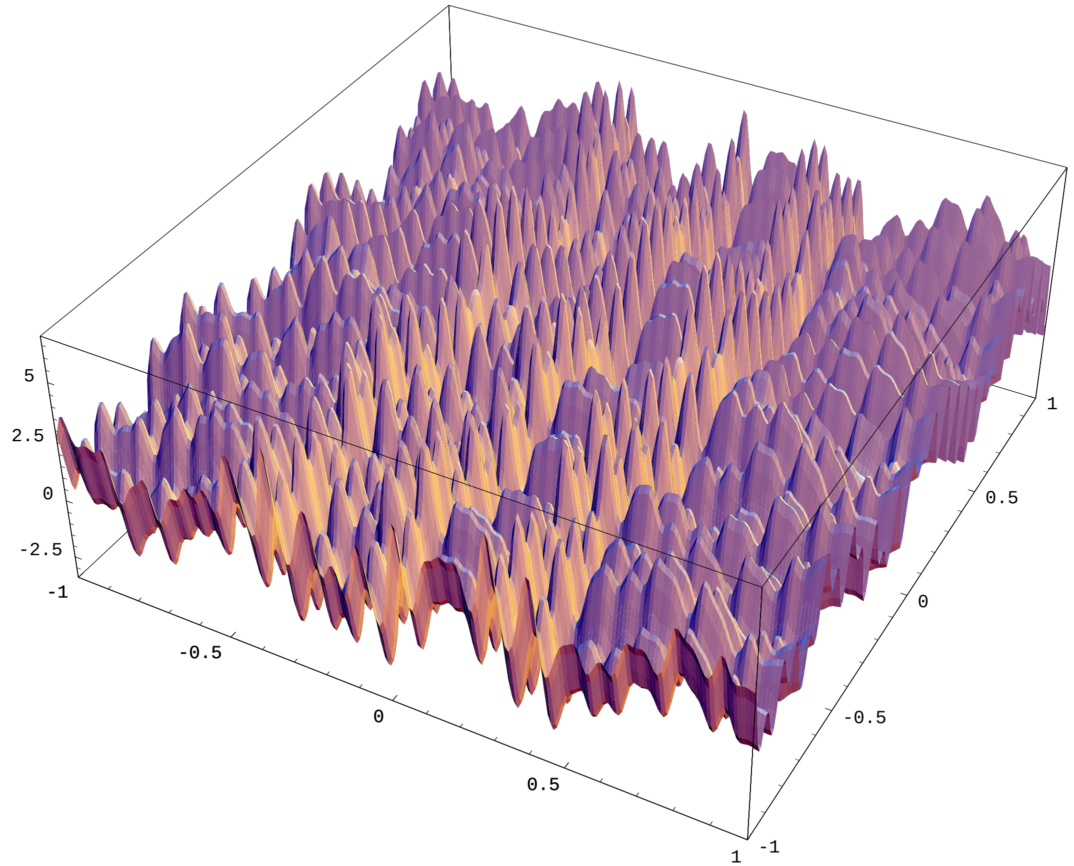
Results and Discussion (Cont'd)

- Problem 2: Parameter estimation in heat exchanger network model.
- Five unconstrained global optimization problems with 4 parameter variables and $13m$ $(m = 4, 8, 12, 16, 20)$ state variables.
- LP solver uses sparse linear algebra.

		I-N tests/CPU time (s)	
m	Variables	HP/RP	LISS_LP
4	56	1/0.12	2/0.27
8	108	375/211.8	44/38.1
12	160	363/498.6	299/346.0
16	212	188/645.8	83/316.8
20	264	220/1357.3	81/504.9

Results and Discussion (Cont'd)

- Trefethen Challenge Problem #4 — Find the Global Minimum



$f(x, y) = \exp(\sin(50x)) + \sin(60\exp(y)) + \sin(70\sin(x)) + \sin(\sin(80y)) - \sin(10(x + y)) + (x^2 + y^2)/4; \quad x \in [-1, 1]; \quad y \in [-1, 1]$

Results and Discussion (Cont'd)

- Solution

$$x \in [-0.02440307969437517, -0.02440307969437516]$$

$$y \in [0.2106124271553557, 0.2106124271553558]$$

$$f \in [-3.306868647475245, -3.306868647475232]$$

- Global minimum is easily found using interval approach

	HP	LISS_LP
I-N tests	1814	1179
CPU time (s)	0.15	0.16

- On relatively easy problems, LP-based strategy is not needed, but still can be used without significant loss of efficiency due to LP overhead.

Concluding Remarks

- An LP-based method can be used to solve the linear interval system arising in the context of the interval-Newton approach for nonlinear equation solving and global optimization.
- The method can obtain tighter bounds on the solution set than standard methods, and thus lead to a large reduction in the number of subintervals that must be tested during the interval-Newton procedure.
- The overhead required to solve the LP subproblems may lead to relatively smaller improvements in overall computation time.
- The interval methodology is a powerful approach for deterministic global optimization.

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