Reliable Nonlinear Parameter Estimation Using Interval Analysis: Error-in-Variable Approach

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Summary

- The objective function in nonlinear parameter estimation problems may have multiple local optima.

- Standard methods for parameter estimation are local methods that provide no guarantee that the global optimum, and thus the best set of model parameters, has been found.

- Interval analysis provides a mathematically and computationally guaranteed method for reliably solving parameter estimation problems, finding the globally optimal parameter values.

- This is demonstrated using three example problems:
  - Vapor-liquid equilibrium model
  - CSTR model
  - Batch reaction kinetics model

Background—Parameter Estimation

- “Standard” approach
  - A distinction is made between dependent and independent variables.
  - It is assumed there are no measurement errors in the independent variables.
  - Result is an estimate of the parameter vector.

- “Error-in-variable” (EIV) approach
  - Measurement errors in all (dependent and independent) variables are taken into account.
  - Result is an estimate of the parameter vector, and of the “true” values of the measured variables.
  - Simultaneous parameter estimation and data reconciliation.

Parameter Estimation (cont'd)

- Measurements $\mathbf{z}_i = (z_{i1}, ..., z_{in})^{\mathrm{T}}$ from $i = 1, \ldots, m$ experiments are available.

- Measurements are to be fit to a model (p equations) of the form $\mathbf{f}(\boldsymbol{\theta}, \mathbf{z}) = \mathbf{0}$, where $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_q)^{\mathrm{T}}$ is an unknown parameter vector.

- There is a vector of measurement errors $\mathbf{e}_i = \tilde{\mathbf{z}}_i - \mathbf{z}_i$, $i = 1, \ldots, m$, that reflects the difference between the measured values $\mathbf{z}_i$ and the unknown "true" values $\tilde{\mathbf{z}}_i$.

- The standard deviation associated with the measurement of variable j is σ_j.

Parameter Estimation (cont'd)

- Using a maximum likelihood estimation with usual assumptions, the EIV parameter estimation problem is

$$\min_{\boldsymbol{\theta}, \tilde{\mathbf{z}}_i} \sum_{i=1}^{m} \sum_{j=1}^{n} \frac{(\tilde{z}_{ij} - z_{ij})^2}{\sigma_j^2}$$

  subject to the model constraints

$$\mathbf{f}(\boldsymbol{\theta}, \tilde{\mathbf{z}}_i) = \mathbf{0}, \quad i = 1, \ldots, m.$$

- This is an $(nm + q)$-variable optimization problem.

- Since optimization is over both $\boldsymbol{\theta}$ and $\tilde{\mathbf{z}}_i$, $i = 1, \ldots, m$, this is likely to be a nonlinear optimization problem even for models that are linear in the parameters.

Parameter Estimation (cont'd)

- If the p model equations can be used to solve algebraically for p of the n variables, then an unconstrained formulation can be used

$$\min_{\boldsymbol{\theta}, \tilde{\mathbf{v}}_i} \ \phi(\boldsymbol{\theta}, \tilde{\mathbf{v}}_i)$$

- $\tilde{\mathbf{v}}_i$, $i = 1, \ldots, m$, refers to the $n - p$ variables not eliminated using the model equations.

- $\phi(\boldsymbol{\theta}, \tilde{\mathbf{v}}_i)$ is the previous objective function after elimination of the p variables by substitution.

- Could solve by seeking stationary points: Solve $\mathbf{g}(\mathbf{y}) \equiv \nabla\phi(\mathbf{y}) = \mathbf{0}$, where $\mathbf{y} = (\boldsymbol{\theta}, \tilde{\mathbf{v}}_i)^{\mathrm{T}}$.

Solution Methods

- Various local methods have been used.
  - SQP (for constrained formulation)
  - Broyden (for unconstrained formulation)
  - Etc.

- Since most EIV optimization problems are nonlinear, and many may be nonconvex, local methods may not find the global optimum.

- Esposito and Floudas (1998) apply a powerful global optimization technique using branch-and-bound with convex underestimators.

Solution Methods (cont'd)

- An alternative is the use of interval analysis, in particular an Interval-Newton/Generalized Bisection (IN/GB) approach.

  - For unconstrained formulation, IN/GB can be used to find (enclose) **all** roots of $\mathbf{g}(\mathbf{y}) = \mathbf{0}$; that is, to find **all** stationary points.

  - For constrained formulation, IN/GB can be used to find (enclose) **all** KKT points.

  - IN/GB can be combined with branch-and-bound so that stationary points or KKT points that cannot be the global minimum need not be found.

Background—Interval Analysis

- A real interval $X = [a, b] = \{x \in \Re \mid a \leq x \leq b\}$ is a segment on the real number line and an interval vector $\mathbf{X} = (X_1, X_2, ..., X_n)^T$ is an n-dimensional rectangle or “box”.

- Basic interval arithmetic for $X = [a, b]$ and $Y = [c, d]$ is X op $Y = \{x \text{ op } y \mid x \in X,\ y \in Y\}$ where op $\in \{+, -, \times, \div\}$. For example, $X + Y = [a + c, b + d]$.

- Interval elementary functions (e.g. $\exp(X)$, $\log(X)$, etc.) are also available.

- Computed endpoints are **rounded out** to guarantee the enclosure.

- The interval extension $F(\mathbf{X})$ encloses all values of $f(\mathbf{x})$ for $\mathbf{x} \in \mathbf{X}$.

- Interval extensions can be computed using interval arithmetic (the “natural” interval extension), or with other techniques.

Interval Approach for Problem Solving

- Interval Newton/Generalized Bisection (IN/GB)
  - Given a system of equations to solve and an initial interval (bounds on all variables):
  - IN/GB can find (enclose) with mathematical and computational certainty either all solutions or determine that no solutions exist. (e.g., Kearfott, 1996; Neumaier, 1990)

- A general purpose approach: requires no simplifying assumptions or problem reformulations

Interval Approach (Cont'd)

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

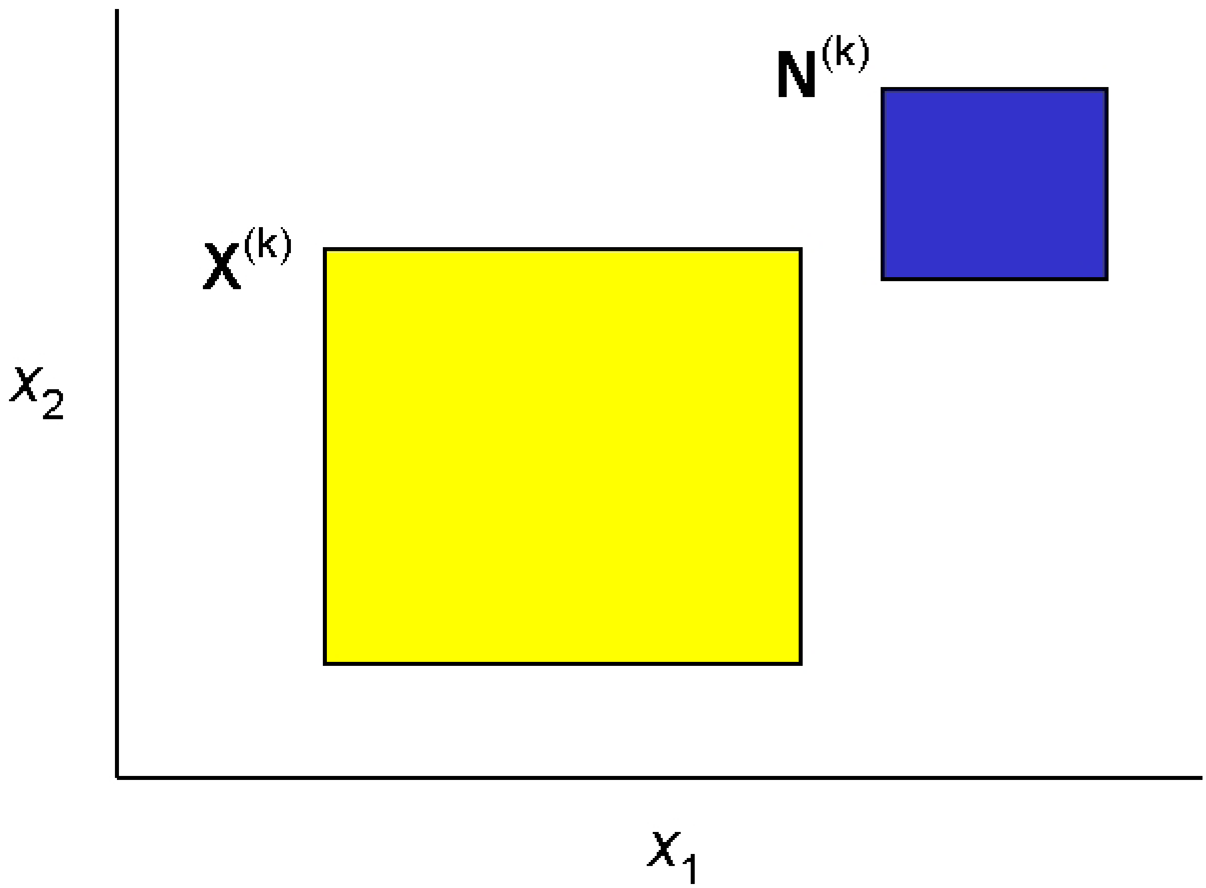
Basic iteration scheme: For a particular subinterval (box), $\mathbf{X}^{(k)}$, arising from some branching (bisection) scheme, perform root inclusion test:

- Compute the interval extension (range) of each function in the system.
- If 0 is not an element of each range, delete (prune) the box.
- If 0 is an element of each range, then compute the *image*, $\mathbf{N}^{(k)}$, of the box by solving the interval Newton equation

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

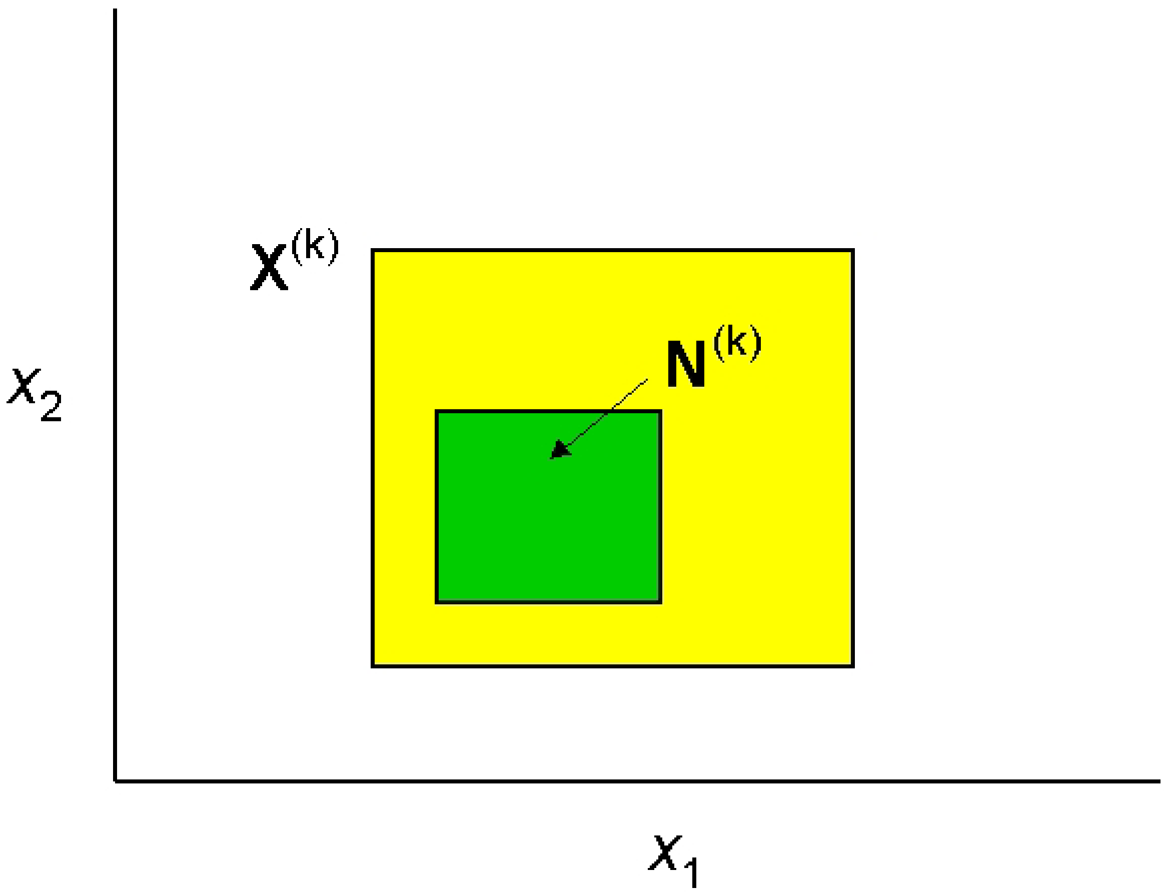
- $\mathbf{x}^{(k)}$ is some point in the interior of $\mathbf{X}^{(k)}$.
- $F'\left(\mathbf{X}^{(k)}\right)$ is an interval extension of the Jacobian of $\mathbf{f}(\mathbf{x})$ over the box $\mathbf{X}^{(k)}$.

Interval Newton Method



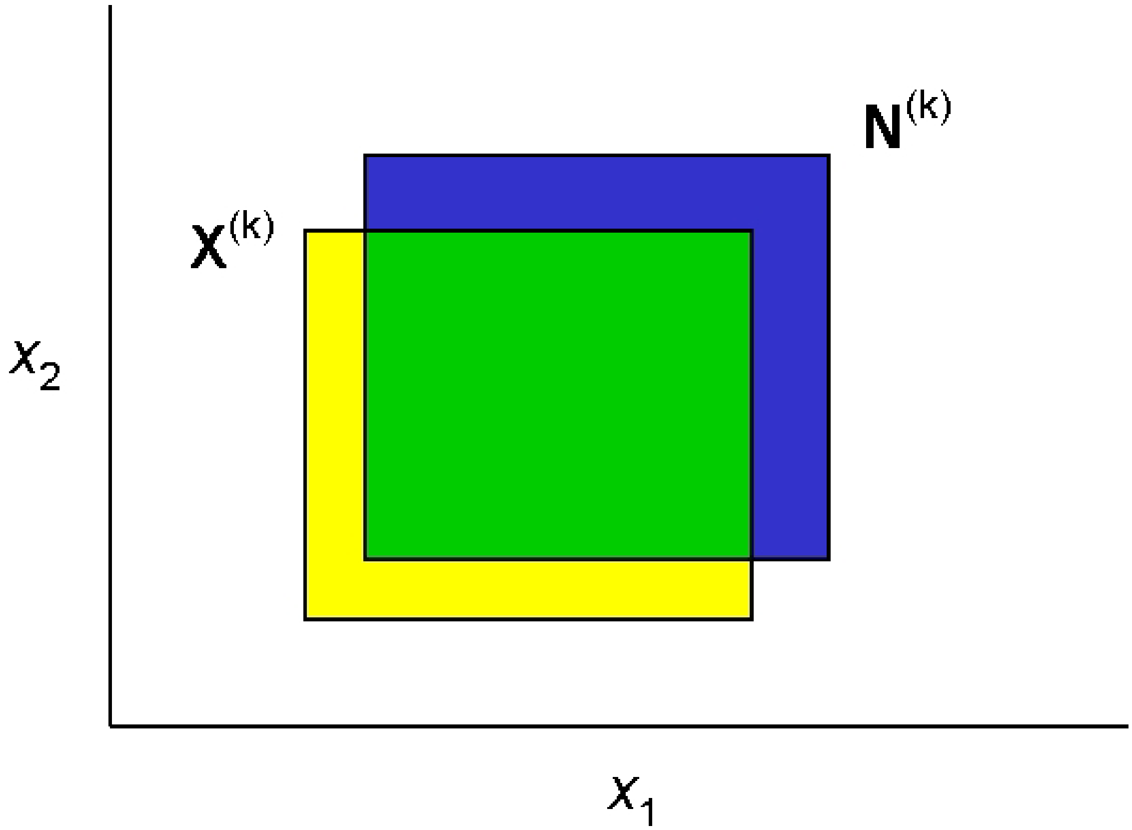
- There is no solution in $\mathbf{X}^{(k)}$.

Interval Newton Method



- There is a *unique* solution in $\mathbf{X}^{(k)}$.
- This solution is in $\mathbf{N}^{(k)}$.
- Point Newton method will converge to solution.

Interval Newton Method



- 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 Approach (Cont'd)

- This is a branch-and-prune scheme on a binary tree.
- No strong assumptions about the function $\mathbf{f}(\mathbf{x})$ need be made.
- The problem $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ must have a finite number of real roots in the given initial interval.
- The method is not suitable if $\mathbf{f}(\mathbf{x})$ is a "black-box" function.
- If there is a solution at a singular point, then existence and uniqueness cannot be confirmed. The eventual result of the IN/GB approach will be a very narrow enclosure that *may* contain one or more solutions.

Interval Approach (Cont'd)

- Can be extended to global optimization problems.

- For unconstrained problems, solve for stationary points.

- For constrained problems, solve for KKT points (or more generally for Fritz-John points).

- Add an additional pruning condition (objective range test):
  - Compute interval extension (range) of objective function.
  - If its lower bound is greater than a known upper bound on the global minimum, prune this subinterval since it cannot contain the global minimum.

- This combines IN/GB with a branch-and-bound scheme.

Problem 1

- Estimation of Van Laar parameters from VLE data (Kim et al., 1990; Esposito and Floudas, 1998).

$$P = \gamma_1 x_1 p_1^0(T) + \gamma_2(1 - x_1)p_2^0(T)$$

$$y_1 = \frac{\gamma_1 x_1 p_1^0(T)}{\gamma_1 x_1 p_1^0(T) + \gamma_2(1 - x_1)p_2^0(T)}$$

where

$$p_1^0(T) = \exp\left[18.5875 - \frac{3626.55}{T - 34.29}\right]$$

$$p_2^0(T) = \exp\left[16.1764 - \frac{2927.17}{T - 50.22}\right]$$

and

$$\gamma_1 = \exp\left[\frac{A}{RT}\left(1 + \frac{A}{B}\frac{x_1}{1 - x_1}\right)^{-2}\right]$$

$$\gamma_2 = \exp\left[\frac{B}{RT}\left(1 + \frac{B}{A}\frac{1 - x_1}{x_1}\right)^{-2}\right] .$$

- There are five data points and four measured variables with two parameters to be determined.

Problem 1 (cont'd)

- Unconstrained formulation is a 12-variable optimization problem.
- Same search space used as in Esposito and Floudas ($\pm 3\sigma$ for the data variables).
- Global optimum found using interval method in 807.9 seconds on Sun Ultra 2/1300 workstation (SPECfp95 = 15.5).
- Same as result found by Esposito and Floudas in 1625 seconds on HP 9000/C160 workstation (SPECfp95 = 16.3).
- By turning off objective range test, can use interval method to show that there is only one stationary point (the global optimum) in the specified initial interval.

Problem 2

- Estimation of parameters in CSTR model (Kim et al., 1990; Esposito and Floudas, 1998).

- Reaction is $\mathrm{A} \xrightarrow{\mathrm{k}_1} \mathrm{B}$.

$$\frac{1}{\tau}(A_0 - A) - k_1 A = 0$$

$$\frac{-B}{\tau} + k_1 A = 0$$

$$\frac{1}{\tau}(T_0 - T) + \frac{-\Delta H_\mathrm{r}}{\rho C_\mathrm{p}}(k_1 A) = 0$$

where

$$k_1 = c_1 \exp\left(\frac{-Q_1}{RT}\right)$$

- There are ten data points and five measured variables with two parameters to be determined.

Problem 2 (cont'd)

- Unconstrained formulation is a 22-variable optimization problem.

- Same search space used as in Esposito and Floudas ($\pm 3\sigma$ for the data variables).

- Global optimum found using interval method in 28.8 seconds on Sun Ultra 2/1300 workstation (SPECfp95 = 15.5).

- Same as result found by Esposito and Floudas in 282.2 seconds on HP 9000/C160 workstation (SPECfp95 = 16.3).

- By turning off objective range test, can use interval method to show that there is only one stationary point (the global optimum) in the specified initial interval.

Problem 3

- Estimation of parameters in batch reaction kinetics model (Bard, 1974).

- Reaction is $\mathrm{A} \xrightarrow{\mathrm{k}} \mathrm{B}$.

$$y = \exp(-kt)$$

where

$$k = \theta_1 \exp\left(-\frac{\theta_2}{T}\right).$$

- There are seven data points (data set 2) and three measured variables with two parameters to be determined.

Problem 3 (cont'd)

- Unconstrained formulation is a 16-variable optimization problem.

- Global optimum found using interval method in 100.5 seconds on Sun Ultra 2/1300 workstation.

- By turning off objective range test, can use interval method to show that there is another local minimum in the specified initial interval.

  – Global minimum: $\theta_1 = 336.474$ h^{-1} and $\theta_2 = 870.757$ K, with $\phi = 34.24904$.

  – Local minimum: $\theta_1 = 7575.339$ h^{-1} and $\theta_2 = 1494.218$ K, with $\phi = 36.46666$.

Problem 3 (cont'd)

- Use results of parameter estimation for prediction of initial reaction rate at 100 K.
- With globally optimal parameters, initial reaction rate at 100 K is 0.0556 h^{-1}.
- With locally optimal parameters, initial reaction rate at 100 K is 0.0025 h^{-1}.
- If a local optimizer was used on this problem, and it converged to the local, but not global, solution, and those results were used for reactor design studies, the results could be dangerously incorrect.

Concluding Remarks

- We have demonstrated a powerful new general-purpose and model-independent approach for solving EIV parameter estimation problems, providing a mathematical and computational guarantee of reliability.

- The guaranteed reliability comes at the expense of a significant CPU requirement. Thus, there is a choice between fast local methods that are not completely reliable, or a slower method that is guaranteed to give the correct answer.

- Continuing advances in hardware and software (e.g., compiler support for interval arithmetic) will make this approach even more attractive.

- Interval analysis provides powerful problem solving techniques with many other applications in the modeling of thermodynamics and phase behavior and in other process modeling problems.

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For more information:

- Contact Prof. Stadtherr at markst@nd.edu
- See also

  http://www.nd.edu/˜markst