



Mathematically  
Rigorous Feasible  
Points

Background  
Motivation and Scope  
Main Ideas  
Experimental Results  
Additional  
Observations

# Some Observations on Exclusion Regions in Interval Branch and Bound Algorithms

Ralph Baker Kearfott

Department of Mathematics  
University of Louisiana at Lafayette

SCAN 2014, September, 2014



Mathematically  
Rigorous Feasible  
Points

# Outline

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional Observations



# Overall Context

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ In branch and bound (B&B) algorithms for constrained global optimization, an acceleration technique is to construct regions  $\mathbf{x}^*$  around local optimizing points  $\check{\mathbf{x}}$ , then delete these *exclusion regions* from further search.



# Overall Context

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ In branch and bound (B&B) algorithms for constrained global optimization, an acceleration technique is to construct regions  $\mathbf{x}^*$  around local optimizing points  $\check{\mathbf{x}}$ , then delete these *exclusion regions* from further search.
- ▶  $\mathbf{x}^*$  too small  $\implies$  adjacent regions not easily rejected. In this case, the B&B algorithm may produce a large *cluster* of small boxes sharing a boundary with  $\mathbf{x}^*$ .



# Overall Context

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ In branch and bound (B&B) algorithms for constrained global optimization, an acceleration technique is to construct regions  $\mathbf{x}^*$  around local optimizing points  $\check{\mathbf{x}}$ , then delete these *exclusion regions* from further search.
- ▶  $\mathbf{x}^*$  too small  $\implies$  adjacent regions not easily rejected. In this case, the B&B algorithm may produce a large *cluster* of small boxes sharing a boundary with  $\mathbf{x}^*$ .
- ▶  $\mathbf{x}^*$  too large  $\implies$  solution bounds are not accurate.



# History

(selected work)

- ▶ Rump (1994 and probably earlier) proposes using interval slopes to construct a small box in which a unique solution exists and, with *epsilon-inflation*, a large box in which no other solutions can exist.

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



# History

(selected work)

- ▶ Rump (1994 and probably earlier) proposes using interval slopes to construct a small box in which a unique solution exists and, with *epsilon-inflation*, a large box in which no other solutions can exist.
- ▶ Kearfott (Math. Comp., 1987) analyzes an abstract B&B algorithm for nonlinear systems, proving under certain conditions that if the diameter of  $\mathbf{x}^*$  is proportional to  $\sqrt{\epsilon}$ , where  $\epsilon$  is the smallest box diameter produced in branch and bound, then clustering of boxes will not occur.

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



# History

(selected work)

- ▶ Rump (1994 and probably earlier) proposes using interval slopes to construct a small box in which a unique solution exists and, with *epsilon-inflation*, a large box in which no other solutions can exist.
- ▶ Kearfott (Math. Comp., 1987) analyzes an abstract B&B algorithm for nonlinear systems, proving under certain conditions that if the diameter of  $\mathbf{x}^*$  is proportional to  $\sqrt{\epsilon}$ , where  $\epsilon$  is the smallest box diameter produced in branch and bound, then clustering of boxes will not occur.
- ▶ Mayer (1995) surveys epsilon-inflation techniques.

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations





# History

(selected work)

- ▶ Rump (1994 and probably earlier) proposes using interval slopes to construct a small box in which a unique solution exists and, with *epsilon-inflation*, a large box in which no other solutions can exist.
- ▶ Kearfott (Math. Comp., 1987) analyzes an abstract B&B algorithm for nonlinear systems, proving under certain conditions that if the diameter of  $\mathbf{x}^*$  is proportional to  $\sqrt{\epsilon}$ , where  $\epsilon$  is the smallest box diameter produced in branch and bound, then clustering of boxes will not occur.
- ▶ Mayer (1995) surveys epsilon-inflation techniques.
- ▶ van Iwaarden (1996, Ph.D. dissertation) independently discovers a technique he calls *backboxing* to construct exclusion regions

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



# History

(selected work)

- ▶ Rump (1994 and probably earlier) proposes using interval slopes to construct a small box in which a unique solution exists and, with *epsilon-inflation*, a large box in which no other solutions can exist.
- ▶ Kearfott (Math. Comp., 1987) analyzes an abstract B&B algorithm for nonlinear systems, proving under certain conditions that if the diameter of  $\mathbf{x}^*$  is proportional to  $\sqrt{\epsilon}$ , where  $\epsilon$  is the smallest box diameter produced in branch and bound, then clustering of boxes will not occur.
- ▶ Mayer (1995) surveys epsilon-inflation techniques.
- ▶ van Iwaarden (1996, Ph.D. dissertation) independently discovers a technique he calls *backboxing* to construct exclusion regions
- ▶ Schichl and Neumaier (2004, SINUM) study using higher order information for constructing exclusion

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



Mathematically  
Rigorous Feasible  
Points

# History

(continued)

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ Schichl and Neumaier (2013, accepted), study exclusion regions for optimization problems.



# History

(continued)

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ Schichl and Neumaier (2013, accepted), study exclusion regions for optimization problems.
- ▶ Domes and Neumaier (March, 2014) propose a new technique for verification of feasibility, for construction of exclusion regions.



# Scope of This Work

## Contrast with Previous Work

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ Previous work depended on uniqueness verification using Kuhn–Tucker conditions and interval Newton methods, or more sophisticated higher-order methods (in the case of pure nonlinear systems, especially).
- ▶ Motivation for this work is to imagine what conditions are necessary in a branch and bound algorithm for boxes adjacent to a small solution-containing box to be verified feasible, then construct the solution-containing box in such a way that adjacent boxes are sure to be verified infeasible. The exclusion region is then constructed to fit exactly this imagined set of adjacent boxes, eliminating the need for them to be created and processed by branch-and-bound.



Mathematically  
Rigorous Feasible  
Points

# The Present Work

## Similarities with Other Ongoing Work

- ▶ This work involves taking a linear combination of the constraints that is likely to be easy to prove infeasible.

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



Mathematically  
Rigorous Feasible  
Points

# The Present Work

## Similarities with Other Ongoing Work

- ▶ This work involves taking a linear combination of the constraints that is likely to be easy to prove infeasible.
- ▶ Work in progress by Domes and Neumaier also takes linear combinations of constraints, but a different linear combination related to approximate Lagrange multipliers.

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



Mathematically  
Rigorous Feasible  
Points

# The Present Work

## Similarities with Other Ongoing Work

- ▶ This work involves taking a linear combination of the constraints that is likely to be easy to prove infeasible.
- ▶ Work in progress by Domes and Neumaier also takes linear combinations of constraints, but a different linear combination related to approximate Lagrange multipliers.
- ▶ The Domes / Neumaier work provides a rejection criterion, while this work provides an exclusion region construction criterion.

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations





Mathematically  
Rigorous Feasible  
Points

# The Present Work

## Similarities with Other Ongoing Work

- ▶ This work involves taking a linear combination of the constraints that is likely to be easy to prove infeasible.
- ▶ Work in progress by Domes and Neumaier also takes linear combinations of constraints, but a different linear combination related to approximate Lagrange multipliers.
- ▶ The Domes / Neumaier work provides a rejection criterion, while this work provides an exclusion region construction criterion.
- ▶ We are also working on use of a third linear combination, for use in a rejection criterion.

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



Mathematically  
Rigorous Feasible  
Points

# The Present Work

## Similarities with Other Ongoing Work

Background

Motivation and Scope

Main Ideas

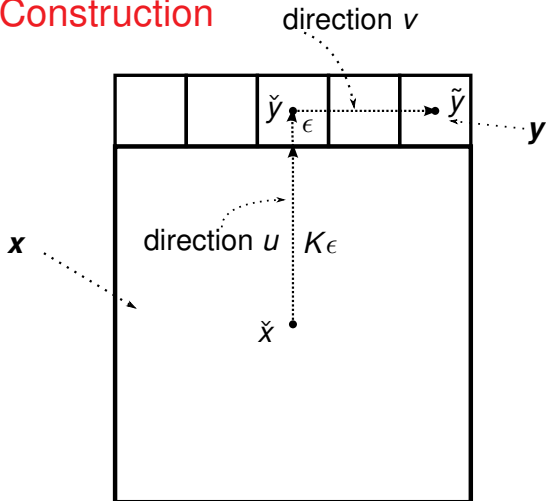
Experimental Results

Additional  
Observations

- ▶ This work involves taking a linear combination of the constraints that is likely to be easy to prove infeasible.
- ▶ Work in progress by Domes and Neumaier also takes linear combinations of constraints, but a different linear combination related to approximate Lagrange multipliers.
- ▶ The Domes / Neumaier work provides a rejection criterion, while this work provides an exclusion region construction criterion.
- ▶ We are also working on use of a third linear combination, for use in a rejection criterion.
- ▶ None of these is a catch-all to work on all problems.



## The Construction



For fixed  $\epsilon$ ,  $K$  is chosen so boxes  $y$  will certainly be rejected.



# Overall Analysis

Mathematically  
Rigorous Feasible  
Points

- ▶ The problem is assumed to have been converted to one with equality constraints only\*.

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

\* *Inequality constraints may also be included later, at some additional complication.*



## Overall Analysis

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ The problem is assumed to have been converted to one with equality constraints only\*.
- ▶ We expand an equality constraint in a Taylor series, and look at increments in a constraint proceeding from the center  $\check{x}$  to the boundary of the central box in a direction  $u$  orthogonal to the box face.

\* *Inequality constraints may also be included later, at some additional complication.*



## Overall Analysis

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ The problem is assumed to have been converted to one with equality constraints only\*.
- ▶ We expand an equality constraint in a Taylor series, and look at increments in a constraint proceeding from the center  $\check{x}$  to the boundary of the central box in a direction  $u$  orthogonal to the box face.
- ▶ We subtract from that possible decrements in directions parallel to the box face.

\* *Inequality constraints may also be included later, at some additional complication.*



## Overall Analysis

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ The problem is assumed to have been converted to one with equality constraints only\*.
- ▶ We expand an equality constraint in a Taylor series, and look at increments in a constraint proceeding from the center  $\check{x}$  to the boundary of the central box in a direction  $u$  orthogonal to the box face.
- ▶ We subtract from that possible decrements in directions parallel to the box face.
- ▶ We bound the increments and decrements with interval evaluations, to prove the constraint is infeasible on a shell abutting the box.

\* *Inequality constraints may also be included later, at some additional complication.*



# Problem Notation

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

**Main Ideas**

Experimental Results

Additional  
Observations





# Problem Notation

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

**Main Ideas**

Experimental Results

Additional  
Observations

minimize  $\varphi(x)$

subject to:

$$C(x) = (c_1(x), \dots, c_{m_1}(x)) = 0,$$

where  $\varphi : \mathbb{R}^n \rightarrow \mathbb{R}$  and

$c_i : \mathbb{R}^n \rightarrow \mathbb{R}, i = 1, \dots, m_1$ .



# Problem Notation

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

minimize  $\varphi(x)$

subject to:

$$C(x) = (c_1(x), \dots, c_{m_1}(x)) = 0,$$

where  $\varphi : \mathbb{R}^n \rightarrow \mathbb{R}$  and

$$c_i : \mathbb{R}^n \rightarrow \mathbb{R}, i = 1, \dots, m_1.$$

The technique will work best if  $\varphi$  is simple, such as if  $\varphi$  consists of a single independent variable.



# Selecting the Constraint

Mathematically  
Rigorous Feasible  
Points

- ▶ A separate constraint combination is used for each coordinate direction  $u$ .

Background

Motivation and Scope

**Main Ideas**

Experimental Results

Additional  
Observations



## Selecting the Constraint

Mathematically  
Rigorous Feasible  
Points

- ▶ A separate constraint combination is used for each coordinate direction  $u$ .
- ▶ The idea is to maximize the rate of change in the direction  $u$  and minimize the rate of change in orthogonal directions.

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



## Selecting the Constraint

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ A separate constraint combination is used for each coordinate direction  $u$ .
- ▶ The idea is to maximize the rate of change in the direction  $u$  and minimize the rate of change in orthogonal directions.
- ▶ The heuristic we use here to achieve this is to choose that constraint combination

$$\tilde{c}_i = \sum_{j=1}^{m_1} \alpha_j c_j(x) \quad \text{which minimizes } \|(\nabla C(\check{x}))\alpha - e_i\|_2$$

over the parameters  $\alpha = (\alpha_1, \dots, \alpha_{m_1})$ , where  $\nabla C(\check{x})$  is the  $n$  by  $m_1$  matrix whose  $i$ -th column is the gradient of  $c_i$  at  $\check{x}$  and where  $e_i \in \mathbb{R}^n$  is the  $i$ -th coordinate vector.



Mathematically  
Rigorous Feasible  
Points

# Computing the Optimal Constraint Combination

## Observations

Background

Motivation and Scope

**Main Ideas**

Experimental Results

Additional  
Observations

- ▶ Minimizing  $\|(\nabla C(\check{x}))_{\alpha} - e_j\|_2$  is a floating point linear least squares problem, that can be done approximately.



Mathematically  
Rigorous Feasible  
Points

# Computing the Optimal Constraint Combination

## Observations

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ Minimizing  $\|(\nabla C(\check{x}))_{\alpha} - e_j\|_2$  is a floating point linear least squares problem, that can be done approximately.
- ▶ High-quality library software for efficiently doing this is available.



Mathematically  
Rigorous Feasible  
Points

# Computing the Optimal Constraint Combination

## Observations

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ Minimizing  $\|(\nabla C(\check{x}))_{\alpha} - e_i\|_2$  is a floating point linear least squares problem, that can be done approximately.
- ▶ High-quality library software for efficiently doing this is available.
- ▶ Once the optimal  $\check{c}_i$  is obtain, we use it to compute an expansion factor  $K_i$  (depending on  $\epsilon$ ) for the  $i$ -th coordinate direction.





# Computing an Overall Expansion Factor $\bar{K}$

Mathematically  
Rigorous Feasible  
Points

- ▶ It is in general not possible to compute box width factors  $K_j$  for each coordinate direction, even with optimal  $\tilde{c}_j$ .

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



# Computing an Overall Expansion Factor $\bar{K}$

Mathematically  
Rigorous Feasible  
Points

- ▶ It is in general not possible to compute box width factors  $K_i$  for each coordinate direction, even with optimal  $\tilde{c}_j$ .
- ▶ The boundary-box rejection criterion depends on each coordinate width, not just the  $i$ -th.

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations



Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

## Computing an Overall Expansion Factor $\bar{K}$

- ▶ It is in general not possible to compute box width factors  $K_i$  for each coordinate direction, even with optimal  $\tilde{c}_j$ .
- ▶ The boundary-box rejection criterion depends on each coordinate width, not just the  $i$ -th.
- ▶ We combine the expansion factors  $K_i$  of reasonable width to an overall expansion factor, used for every coordinate:

$$\bar{K} = \begin{cases} \max_{\substack{1 \leq i \leq n, p \in \{-1, 1\} \\ K_{i,p} < K_{\max}}} K_{i,p} & \text{if } \exists K_{i,p} < K_{\max}, \\ K_{\max} & \text{otherwise.} \end{cases}$$

$\bar{K}_\epsilon$  will be the radius of the central box in each coordinate direction.



# Experimental Setup

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ We implemented the techniques using libraries from GlobSol.



# Experimental Setup

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ We implemented the techniques using libraries from GlobSol.
- ▶ We tried the techniques on a subset of the COCONUT Lib-1 test set.



# Experimental Setup

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ We implemented the techniques using libraries from GlobSol.
- ▶ We tried the techniques on a subset of the COCONUT Lib-1 test set.
- ▶ We automatically converted the inequality constraints to equality constraints with bound constraints, for these problems.



# Experimental Setup

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ We implemented the techniques using libraries from GlobSol.
- ▶ We tried the techniques on a subset of the COCONUT Lib-1 test set.
- ▶ We automatically converted the inequality constraints to equality constraints with bound constraints, for these problems.
- ▶ For each problem, we measured the number of faces of the central box upon which adjacent small boxes can be eliminated.



# Experimental Results

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

**Experimental Results**

Additional  
Observations

- ▶ Of 26 problems tried, 15 had faces upon which adjacent small boxes could be eliminated.





# Experimental Results

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

**Experimental Results**

Additional  
Observations

- ▶ Of 26 problems tried, 15 had faces upon which adjacent small boxes could be eliminated.
- ▶ Of the problems with box faces upon which adjacent small boxes could be eliminated, the number of faces ranged from  $1/34$  to  $32/44$ .



## Additional Observations

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ The use of interval-valued partial derivatives in a Taylor expansion is similar to what is done in the interval Gauss–Seidel method.



## Additional Observations

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ The use of interval-valued partial derivatives in a Taylor expansion is similar to what is done in the interval Gauss–Seidel method.
- ▶ The linear combination of constraints is a kind of preconditioner for the system of constraints.



## Additional Observations

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ The use of interval-valued partial derivatives in a Taylor expansion is similar to what is done in the interval Gauss–Seidel method.
- ▶ The linear combination of constraints is a kind of preconditioner for the system of constraints.
- ▶ We are presently investigating an alternate linear combination, motivated by the same ideas, for filtering boxes during the branch and bound algorithm.



## Additional Observations

Mathematically  
Rigorous Feasible  
Points

Background

Motivation and Scope

Main Ideas

Experimental Results

Additional  
Observations

- ▶ The use of interval-valued partial derivatives in a Taylor expansion is similar to what is done in the interval Gauss–Seidel method.
- ▶ The linear combination of constraints is a kind of preconditioner for the system of constraints.
- ▶ We are presently investigating an alternate linear combination, motivated by the same ideas, for filtering boxes during the branch and bound algorithm.
- ▶ We are comparing the techniques, theoretically and in practice, to our optimally preconditioned interval Gauss–Seidel method.