Degree Computation and Global Optimization

A Personal Perspective

R. Baker Kearfott

Department of Mathematics
University of Louisiana at Lafayette

Stenger-2007

(slide 2)

Outline

Outline

(slide 4)

Frank's Papers

- Frank Stenger, "An Algorithm for the Topological Degree of a Mapping in $\mathbb{R}^n$," *Numerische Mathematik* **25**, pp. 23–28 (1976).
- F. Stenger and C. Harvey, "A Two-Dimensional Analogue to the Method of Bisections for Solving Nonlinear Equations," *Quarterly Journal of Applied Mathematics* **33, pp. 351–368 (1976).**

Computing the Topological Degree

- The topological degree is a generalization of the *winding number* in complex analysis.
- If $F : \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}^n$ and $\partial\mathcal{D}$ is the boundary of $\mathcal{D}$, then the topological degree $d(F, \partial\mathcal{D})$ can be characterized as the number of times the image of $\partial\mathcal{D}$ under $F/\|F\|$ covers $e_1 = (1, 0, \ldots, 0)$ with a positive orientation minus the number of times e_1 is covered with a negative orientation.
- Frank characterized the topological degree as a sum of certain determinants, provided $\partial\mathcal{D}$ is *sufficiently refined*.
- The number of solutions $x^* \in \mathcal{D}$ is equal to $d(F, \partial\mathcal{D})$ mod 2, and is equal to $d(F, \partial\mathcal{D})$ if F represents the real and imaginary parts of an analytic function in $\mathbb{C}^{(n/2)}$.

Computing the Topological Degree

- The topological degree is a generalization of the *winding number* in complex analysis.
- If $F : \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}^n$ and $\partial\mathcal{D}$ is the boundary of $\mathcal{D}$, then the topological degree $d(F, \partial\mathcal{D})$ can be characterized as the number of times the image of $\partial\mathcal{D}$ under $F/\|F\|$ covers $e_1 = (1, 0, \ldots, 0)$ with a positive orientation minus the number of times e_1 is covered with a negative orientation.
- Frank characterized the topological degree as a sum of certain determinants, provided $\partial\mathcal{D}$ is *sufficiently refined*.
- The number of solutions $x^* \in \mathcal{D}$ is equal to $d(F, \partial\mathcal{D})$ mod 2, and is equal to $d(F, \partial\mathcal{D})$ if F represents the real and imaginary parts of an analytic function in $\mathbb{C}^{(n/2)}$.

Computing the Topological Degree

- The topological degree is a generalization of the *winding number* in complex analysis.
- If $F : \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}^n$ and $\partial\mathcal{D}$ is the boundary of $\mathcal{D}$, then the topological degree $d(F, \partial\mathcal{D})$ can be characterized as the number of times the image of $\partial\mathcal{D}$ under $F/\|F\|$ covers $e_1 = (1, 0, \ldots, 0)$ with a positive orientation minus the number of times e_1 is covered with a negative orientation.
- Frank characterized the topological degree as a sum of certain determinants, provided $\partial\mathcal{D}$ is *sufficiently refined*.
- The number of solutions $x^* \in \mathcal{D}$ is equal to $d(F, \partial\mathcal{D})$ mod 2, and is equal to $d(F, \partial\mathcal{D})$ if F represents the real and imaginary parts of an analytic function in $\mathbb{C}^{(n/2)}$.

Computing the Topological Degree

- The topological degree is a generalization of the *winding number* in complex analysis.
- If $F : \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}^n$ and $\partial\mathcal{D}$ is the boundary of $\mathcal{D}$, then the topological degree $d(F, \partial\mathcal{D})$ can be characterized as the number of times the image of $\partial\mathcal{D}$ under $F/\|F\|$ covers $e_1 = (1, 0, \ldots, 0)$ with a positive orientation minus the number of times e_1 is covered with a negative orientation.
- Frank characterized the topological degree as a sum of certain determinants, provided $\partial\mathcal{D}$ is *sufficiently refined*.
- The number of solutions $x^* \in \mathcal{D}$ is equal to $d(F, \partial\mathcal{D})$ mod 2, and is equal to $d(F, \partial\mathcal{D})$ if F represents the real and imaginary parts of an analytic function in $\mathbb{C}^{(n/2)}$.

Outline

1 Frank's Topological Degree Work
- The First Papers
- Kearfott's Dissertation
- Offshoots

2 Problems and Explorations
- On Sufficient Refinement
- Continuation Methods
- Shift of Focus

3 Interval Techniques
- Bounding Ranges
- Proving Existence and Uniqueness
- GlobSol

4 Back to the Topological Degree

Kearfott's Dissertation

- Kearfott developed an alternate formula for $d(F, \partial\mathcal{D})$ that involved counting matrices formed from the algebraic signs of components of F.
- Kearfott also implemented an algorithm for computing $d(F, \partial\mathcal{D})$ for $\mathcal{D} \in \mathbb{R}^n$ based on successive adaptive subdivision of simplexes by bisecting their longest edges.
- In Kearfott's initial algorithm, "sufficient refinement" was determined by a heuristic parameter p: If the contribution of a subregion did not change after p subdivisions, the subregion was deemed to be sufficiently refined.
- Kearfott incorporated the degree computation algorithm efficiently into a generalized bisection algorithm to compute a solution $x^* \in \mathcal{D}$, $F(x^*) = 0$.

Kearfott's Dissertation

- Kearfott developed an alternate formula for $d(F, \partial\mathcal{D})$ that involved counting matrices formed from the algebraic signs of components of F.
- Kearfott also implemented an algorithm for computing $d(F, \partial\mathcal{D})$ for $\mathcal{D} \in \mathbb{R}^n$ based on successive adaptive subdivision of simplexes by bisecting their longest edges.
- In Kearfott's initial algorithm, "sufficient refinement" was determined by a heuristic parameter p: If the contribution of a subregion did not change after p subdivisions, the subregion was deemed to be sufficiently refined.
- Kearfott incorporated the degree computation algorithm efficiently into a generalized bisection algorithm to compute a solution $x^* \in \mathcal{D}$, $F(x^*) = 0$.

Kearfott's Dissertation

- Kearfott developed an alternate formula for $d(F, \partial\mathcal{D})$ that involved counting matrices formed from the algebraic signs of components of F.
- Kearfott also implemented an algorithm for computing $d(F, \partial\mathcal{D})$ for $\mathcal{D} \in \mathbb{R}^n$ based on successive adaptive subdivision of simplexes by bisecting their longest edges.
- In Kearfott's initial algorithm, "sufficient refinement" was determined by a heuristic parameter p: If the contribution of a subregion did not change after p subdivisions, the subregion was deemed to be sufficiently refined.
- Kearfott incorporated the degree computation algorithm efficiently into a generalized bisection algorithm to compute a solution $x^* \in \mathcal{D}$, $F(x^*) = 0$.

Kearfott's Dissertation

- Kearfott developed an alternate formula for $d(F, \partial\mathcal{D})$ that involved counting matrices formed from the algebraic signs of components of F.
- Kearfott also implemented an algorithm for computing $d(F, \partial\mathcal{D})$ for $\mathcal{D} \in \mathbb{R}^n$ based on successive adaptive subdivision of simplexes by bisecting their longest edges.
- In Kearfott's initial algorithm, "sufficient refinement" was determined by a heuristic parameter p: If the contribution of a subregion did not change after p subdivisions, the subregion was deemed to be sufficiently refined.
- Kearfott incorporated the degree computation algorithm efficiently into a generalized bisection algorithm to compute a solution $x^* \in \mathcal{D}$, $F(x^*) = 0$.

The Generalized Method of Bisection

- is basically a *branch and bound* algorithm involving an exhaustive binary search of the entire region;
- is related to adaptive quadrature algorithms;
- is related to similar search algorithms that were being developed separately for various types of optimization problems.

The Generalized Method of Bisection

- is basically a *branch and bound* algorithm involving an exhaustive binary search of the entire region;
- is related to adaptive quadrature algorithms;
- is related to similar search algorithms that were being developed separately for various types of optimization problems.

The Generalized Method of Bisection

- is basically a *branch and bound* algorithm involving an exhaustive binary search of the entire region;
- is related to adaptive quadrature algorithms;
- is related to similar search algorithms that were being developed separately for various types of optimization problems.

Bisection of Simplices

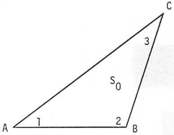


FIGURE 4.5

THE ORIGINAL SIMPLEX

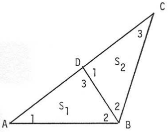


FIGURE 4.6

THE FIRST SUBDIVISION

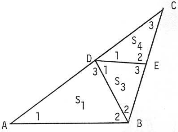


FIGURE 4.7

THE SECOND SUBDIVISION

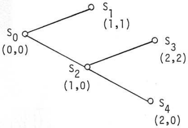


FIGURE 4.8

THE TREE

Foreseen Applications

- **Applications Frank foresaw**
  - Singular problems and non-smooth problems
  - The hidden line problem and other problems in computer graphics

Foreseen Applications

- **Applications Frank foresaw**
  - Singular problems and non-smooth problems
  - The hidden line problem and other problems in computer graphics

Foreseen Applications

- **Applications Frank foresaw**
  - Singular problems and non-smooth problems
  - The hidden line problem and other problems in computer graphics

Outline

Some Offshoots

- **Adaptive subdivision in finite element methods**: the path Martin Stynes took
- **Geometry of subdivision of simplexes**
  - First attempted in Kearfott, "A Proof of Convergence and an Error Bound for the Method of Bisection in $\mathbb{R}^n$," *Math. Comp.* **32**, 144, pp. 1147–1153 (1978).
  - Continued in and completed more definitively in Reiner Horst, "On Generalized Bisection of n-Simplices," *Math. Comp.* **66**, 218, pp. 691–698 (1997).
- **Further developments in computation of and application of the topological degree.**

Some Offshoots

- **Adaptive subdivision in finite element methods**: the path Martin Stynes took
- **Geometry of subdivision of simplexes**
  - First attempted in Kearfott, "A Proof of Convergence and an Error Bound for the Method of Bisection in $\mathbb{R}^n$," *Math. Comp.* **32**, 144, pp. 1147–1153 (1978).
  - Continued in and completed more definitively in Reiner Horst, "On Generalized Bisection of n-Simplices," *Math. Comp.* **66**, 218, pp. 691–698 (1997).
- **Further developments in computation of and application of the topological degree.**

Some Offshoots

- **Adaptive subdivision in finite element methods**: the path Martin Stynes took
- **Geometry of subdivision of simplexes**
  - First attempted in Kearfott, "A Proof of Convergence and an Error Bound for the Method of Bisection in $\mathbb{R}^n$," *Math. Comp.* **32**, 144, pp. 1147–1153 (1978).
  - Continued in and completed more definitively in Reiner Horst, "On Generalized Bisection of n-Simplices," *Math. Comp.* **66**, 218, pp. 691–698 (1997).
- **Further developments in computation of and application of the topological degree.**

Some Offshoots

- **Adaptive subdivision in finite element methods**: the path Martin Stynes took
- **Geometry of subdivision of simplexes**
  - First attempted in Kearfott, "A Proof of Convergence and an Error Bound for the Method of Bisection in $\mathbb{R}^n$," *Math. Comp.* **32**, 144, pp. 1147–1153 (1978).
  - Continued in and completed more definitively in Reiner Horst, "On Generalized Bisection of *n*-Simplices," *Math. Comp.* **66**, 218, pp. 691–698 (1997).
- **Further developments in computation of and application of the topological degree.**

(slide 26)

Some Offshoots

- **Adaptive subdivision in finite element methods**: the path Martin Stynes took
- **Geometry of subdivision of simplexes**
  - First attempted in Kearfott, "A Proof of Convergence and an Error Bound for the Method of Bisection in $\mathbb{R}^n$," *Math. Comp.* **32**, 144, pp. 1147–1153 (1978).
  - Continued in and completed more definitively in Reiner Horst, "On Generalized Bisection of n-Simplices," *Math. Comp.* **66**, 218, pp. 691–698 (1997).
- **Further developments in computation of and application of the topological degree.**

Other Early Work

- Frank and Chris, along with A. Eiger, also continued to work on generalized bisection.
  - Krzysztof Sikorski, "A Three–Dimensional Analogue to the Method of Bisections for Solving Nonlinear Equations," *Math. Comp.* **33**, 146, pp. 722–738 (1979).
  - A. Eiger, K. Sikorski, and F. Stenger, "A Bisection Method for Systems of Nonlinear Equations," *ACM Transactions on Mathematical Software* **10**, 4, pp. 367–377 (1984).
- Chris continued to analyze n-dimensional bisection from a computational complexity point of view. (He has various publications along these lines.)

Other Early Work

- Frank and Chris, along with A. Eiger, also continued to work on generalized bisection.
  - Krzysztof Sikorski, "A Three–Dimensional Analogue to the Method of Bisections for Solving Nonlinear Equations," *Math. Comp.* **33**, 146, pp. 722–738 (1979).
  - A. Eiger, K. Sikorski, and F. Stenger, "A Bisection Method for Systems of Nonlinear Equations," *ACM Transactions on Mathematical Software* **10**, 4, pp. 367–377 (1984).
- Chris continued to analyze *n*-dimensional bisection from a computational complexity point of view. (He has various publications along these lines.)

Other Early Work

- Frank and Chris, along with A. Eiger, also continued to work on generalized bisection.
  - Krzysztof Sikorski, "A Three–Dimensional Analogue to the Method of Bisections for Solving Nonlinear Equations," *Math. Comp.* **33**, 146, pp. 722–738 (1979).
  - A. Eiger, K. Sikorski, and F. Stenger, "A Bisection Method for Systems of Nonlinear Equations," *ACM Transactions on Mathematical Software* **10**, 4, pp. 367–377 (1984).
- Chris continued to analyze n-dimensional bisection from a computational complexity point of view. (He has various publications along these lines.)

Other Early Work

- Frank and Chris, along with A. Eiger, also continued to work on generalized bisection.
  - Krzysztof Sikorski, "A Three–Dimensional Analogue to the Method of Bisections for Solving Nonlinear Equations," *Math. Comp.* **33**, 146, pp. 722–738 (1979).
  - A. Eiger, K. Sikorski, and F. Stenger, "A Bisection Method for Systems of Nonlinear Equations," *ACM Transactions on Mathematical Software* **10**, 4, pp. 367–377 (1984).
- Chris continued to analyze n-dimensional bisection from a computational complexity point of view. (He has various publications along these lines.)

Outline

On Sufficient Refinement

- Combinatorial technicalities aside, sufficient refinement basically occurs when the subdivision is such that at least one component of F has constant sign on each simplex in the subdivision.
- The heuristic checked the signs of components of F at vertices of simplexes in the subdivision only, and failed in practice for many examples.
- Knowing bounds on the ranges of components of F can determine sufficient refinement.
- Sufficient refinement can be rigorously checked if Lipschitz constants or moduli of continuity are known for the components of F.
- A simple way of checking sufficient refinement is by interval evaluations of the components of F over sub-regions.

On Sufficient Refinement

- Combinatorial technicalities aside, sufficient refinement basically occurs when the subdivision is such that at least one component of F has constant sign on each simplex in the subdivision.
- The heuristic checked the signs of components of F at vertices of simplexes in the subdivision only, and failed in practice for many examples.
- Knowing bounds on the ranges of components of F can determine sufficient refinement.
- Sufficient refinement can be rigorously checked if Lipschitz constants or moduli of continuity are known for the components of F.
- A simple way of checking sufficient refinement is by interval evaluations of the components of F over sub-regions.

On Sufficient Refinement

- Combinatorial technicalities aside, sufficient refinement basically occurs when the subdivision is such that at least one component of F has constant sign on each simplex in the subdivision.
- The heuristic checked the signs of components of F at vertices of simplexes in the subdivision only, and failed in practice for many examples.
- Knowing bounds on the ranges of components of F can determine sufficient refinement.
- Sufficient refinement can be rigorously checked if Lipschitz constants or moduli of continuity are known for the components of F.
- A simple way of checking sufficient refinement is by interval evaluations of the components of F over sub-regions.

On Sufficient Refinement

- Combinatorial technicalities aside, sufficient refinement basically occurs when the subdivision is such that at least one component of F has constant sign on each simplex in the subdivision.
- The heuristic checked the signs of components of F at vertices of simplexes in the subdivision only, and failed in practice for many examples.
- Knowing bounds on the ranges of components of F can determine sufficient refinement.
- Sufficient refinement can be rigorously checked if Lipschitz constants or moduli of continuity are known for the components of F.
- A simple way of checking sufficient refinement is by interval evaluations of the components of F over sub-regions.

Outline

Continuation Methods

- (1980's) Simplicial and continuation methods follow a one-dimensional solution set of a parametrized nonlinear system $H(x, \lambda) : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$.
- Such methods can in theory be used to solve $F(x) = 0$ by following paths from zeros of a starting function G to zeros of the target function F.
- Theory states that, for polynomial systems F, the if F is random and the coefficients of G are chosen randomly, the set of coefficients of G for which continuation does not lead to all solutions of $F = 0$ has measure zero.
- In practice, F constructed from science and engineering models is not random, and does not lie on that "set of measure zero."
- In practice, heuristic tolerances in the path-following algorithms often led to jumping across paths, especially in early algorithms.

Continuation Methods

- (1980's) Simplicial and continuation methods follow a one-dimensional solution set of a parametrized nonlinear system $H(x,\lambda) : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$.
- Such methods can in theory be used to solve $F(x) = 0$ by following paths from zeros of a starting function G to zeros of the target function F.
- Theory states that, for polynomial systems F, the if F is random and the coefficients of G are chosen randomly, the set of coefficients of G for which continuation does not lead to all solutions of $F = 0$ has measure zero.
- In practice, F constructed from science and engineering models is not random, and does not lie on that "set of measure zero."
- In practice, heuristic tolerances in the path-following algorithms often led to jumping across paths, especially in early algorithms.

Continuation Methods

- (1980's) Simplicial and continuation methods follow a one-dimensional solution set of a parametrized nonlinear system $H(x, \lambda) : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$.
- Such methods can in theory be used to solve $F(x) = 0$ by following paths from zeros of a starting function G to zeros of the target function F.
- Theory states that, for polynomial systems F, the if F is random and the coefficients of G are chosen randomly, the set of coefficients of G for which continuation does not lead to all solutions of $F = 0$ has measure zero.
- In practice, F constructed from science and engineering models is not random, and does not lie on that "set of measure zero."
- In practice, heuristic tolerances in the path-following algorithms often led to jumping across paths, especially in early algorithms.

Continuation Methods

- (1980's) Simplicial and continuation methods follow a one-dimensional solution set of a parametrized nonlinear system $H(x, \lambda) : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$.
- Such methods can in theory be used to solve $F(x) = 0$ by following paths from zeros of a starting function G to zeros of the target function F.
- Theory states that, for polynomial systems F, the if F is random and the coefficients of G are chosen randomly, the set of coefficients of G for which continuation does not lead to all solutions of $F = 0$ has measure zero.
- In practice, F constructed from science and engineering models is not random, and does not lie on that "set of measure zero."
- In practice, heuristic tolerances in the path-following algorithms often led to jumping across paths, especially in early algorithms.

Continuation Methods

- (1980's) Simplicial and continuation methods follow a one-dimensional solution set of a parametrized nonlinear system $H(x, \lambda) : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$.
- Such methods can in theory be used to solve $F(x) = 0$ by following paths from zeros of a starting function G to zeros of the target function F.
- Theory states that, for polynomial systems F, the if F is random and the coefficients of G are chosen randomly, the set of coefficients of G for which continuation does not lead to all solutions of $F = 0$ has measure zero.
- In practice, F constructed from science and engineering models is not random, and does not lie on that "set of measure zero."
- In practice, heuristic tolerances in the path-following algorithms often led to jumping across paths, especially in early algorithms.

Outline

Initial Tries and Shift of Focus

- Kearfott initially explored various alternate schemes for the computing the degree
  - Recursive reduction of dimension, such as in "A Summary of Recent Experiments to Compute the Topological Degree," in *Applied Nonlinear Analysis*, ed. V. Lakshmikantham, Academic Press, 1979.
  - Use of moduli of continuity and Lipschitz constants to determine sufficient refinement (unpublished).
  - Kearfott was attracted to interval computations since they could give rigorous bounds on ranges with simple function evaluations.
- Kearfott eventually focussed on finding *all* roots, employing interval techniques.

Initial Tries and Shift of Focus

- Kearfott initially explored various alternate schemes for the computing the degree
  - Recursive reduction of dimension, such as in "A Summary of Recent Experiments to Compute the Topological Degree," in *Applied Nonlinear Analysis*, ed. V. Lakshmikantham, Academic Press, 1979.
  - Use of moduli of continuity and Lipschitz constants to determine sufficient refinement (unpublished).
  - Kearfott was attracted to interval computations since they could give rigorous bounds on ranges with simple function evaluations.
- Kearfott eventually focussed on finding *all* roots, employing interval techniques.

Initial Tries and Shift of Focus

- Kearfott initially explored various alternate schemes for the computing the degree
  - Recursive reduction of dimension, such as in "A Summary of Recent Experiments to Compute the Topological Degree," in *Applied Nonlinear Analysis*, ed. V. Lakshmikantham, Academic Press, 1979.
  - Use of moduli of continuity and Lipschitz constants to determine sufficient refinement (unpublished).
  - Kearfott was attracted to interval computations since they could give rigorous bounds on ranges with simple function evaluations.
- Kearfott eventually focussed on finding *all* roots, employing interval techniques.

Initial Tries and Shift of Focus

- Kearfott initially explored various alternate schemes for the computing the degree
  - Recursive reduction of dimension, such as in "A Summary of Recent Experiments to Compute the Topological Degree," in *Applied Nonlinear Analysis*, ed. V. Lakshmikantham, Academic Press, 1979.
  - Use of moduli of continuity and Lipschitz constants to determine sufficient refinement (unpublished).
  - Kearfott was attracted to interval computations since they could give rigorous bounds on ranges with simple function evaluations.
- Kearfott eventually focussed on finding *all* roots, employing interval techniques.

Initial Tries and Shift of Focus

- Kearfott initially explored various alternate schemes for the computing the degree
  - Recursive reduction of dimension, such as in "A Summary of Recent Experiments to Compute the Topological Degree," in *Applied Nonlinear Analysis*, ed. V. Lakshmikantham, Academic Press, 1979.
  - Use of moduli of continuity and Lipschitz constants to determine sufficient refinement (unpublished).
  - Kearfott was attracted to interval computations since they could give rigorous bounds on ranges with simple function evaluations.
- Kearfott eventually focussed on finding *all* roots, employing interval techniques.

Outline

Bounding Ranges with Interval Arithmetic

- Each basic interval operation $\odot \in \{+, -, \times, \div, \text{etc.}\}$ is defined by

$$\boldsymbol{x} \odot \boldsymbol{y} = \{x \odot y \mid x \in \boldsymbol{x} \text{ and } y \in \boldsymbol{y}\}.$$

- This definition can be made operational; for example, for $\boldsymbol{x} = [\underline{x}, \overline{x}]$ and $\boldsymbol{y} = [\underline{y}, \overline{y}]$, $\boldsymbol{x} + \boldsymbol{y} = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$; similarly, ranges of functions such as sin, exp can be computed.
- Evaluation of an expression with this interval arithmetic gives *bounds* on the range of the expression.
- With *directed rounding* (e.g. using IEEE standard arithmetic), the computer can give mathematically rigorous bounds on ranges.

Bounding Ranges with Interval Arithmetic

- Each basic interval operation $\odot \in \{+, -, \times, \div, \text{etc.}\}$ is defined by

$$\boldsymbol{x} \odot \boldsymbol{y} = \{x \odot y \mid x \in \boldsymbol{x} \text{ and } y \in \boldsymbol{y}\}.$$

- This definition can be made operational; for example, for $\boldsymbol{x} = [\underline{x}, \overline{x}]$ and $\boldsymbol{y} = [\underline{y}, \overline{y}]$, $\boldsymbol{x} + \boldsymbol{y} = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$; similarly, ranges of functions such as sin, exp can be computed.
- Evaluation of an expression with this interval arithmetic gives *bounds* on the range of the expression.
- With *directed rounding* (e.g. using IEEE standard arithmetic), the computer can give mathematically rigorous bounds on ranges.

Bounding Ranges with Interval Arithmetic

- Each basic interval operation $\odot \in \{+, -, \times, \div, \text{etc.}\}$ is defined by

$$\boldsymbol{x} \odot \boldsymbol{y} = \{x \odot y \mid x \in \boldsymbol{x} \text{ and } y \in \boldsymbol{y}\}.$$

- This definition can be made operational; for example, for $\boldsymbol{x} = [\underline{x}, \overline{x}]$ and $\boldsymbol{y} = [\underline{y}, \overline{y}]$, $\boldsymbol{x} + \boldsymbol{y} = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$; similarly, ranges of functions such as sin, exp can be computed.
- Evaluation of an expression with this interval arithmetic gives *bounds* on the range of the expression.
- With *directed rounding* (e.g. using IEEE standard arithmetic), the computer can give mathematically rigorous bounds on ranges.

Bounding Ranges with Interval Arithmetic

- Each basic interval operation $\odot \in \{+, -, \times, \div, \text{etc.}\}$ is defined by

$$\boldsymbol{x} \odot \boldsymbol{y} = \{x \odot y \mid x \in \boldsymbol{x} \text{ and } y \in \boldsymbol{y}\}.$$

- This definition can be made operational; for example, for $\boldsymbol{x} = [\underline{x}, \overline{x}]$ and $\boldsymbol{y} = [\underline{y}, \overline{y}]$, $\boldsymbol{x} + \boldsymbol{y} = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$; similarly, ranges of functions such as sin, exp can be computed.
- Evaluation of an expression with this interval arithmetic gives *bounds* on the range of the expression.
- With *directed rounding* (e.g. using IEEE standard arithmetic), the computer can give mathematically rigorous bounds on ranges.

Outline

Proving Existence and Uniqueness

Let $f(x) = 0$, $f: \mathbb{R}^n \to \mathbb{R}^n$ represent a system of nonlinear equations. Think of an interval Newton method as an operator sending $\boldsymbol{x}$ to $\tilde{\boldsymbol{x}}$:

$$\tilde{\boldsymbol{x}} = \boldsymbol{N}(f; \boldsymbol{x}, \check{x}) = \check{x} + \boldsymbol{v}, \quad \text{where} \quad \Sigma\left(\boldsymbol{A}, -f(\check{x})\right) \subset \boldsymbol{v},$$

where $\boldsymbol{A}$ is a Lipschitz matrix for f over $\boldsymbol{x}$ and $\Sigma\left(\boldsymbol{A}, -f(\check{x})\right)$ is that set $\{x \in \mathbb{R}^n\}$ such that there exists an $A \in \boldsymbol{A}$ with $Ax = -f(\check{x})$.

Theorem

Suppose $\tilde{\boldsymbol{x}}$ is the image of $\boldsymbol{x}$ under an interval Newton method. If $\tilde{\boldsymbol{x}} \subseteq \boldsymbol{x}$, it follows that there exists a unique solution of $f(x) = 0$ within $\boldsymbol{x}$.

Interval Newton Methods

A Practical Summary

- $\boldsymbol{N}(f;\boldsymbol{x},\check{x})$ can be computed similarly to a classical point multivariate Newton step, but with interval arithmetic.
- Any solutions of $f(x)=0$ in $\boldsymbol{x}$ must be in $\boldsymbol{N}(f;\boldsymbol{x},\check{x})$. (Hence, an interval Newton can be used to reduce the volume of $\boldsymbol{x}$, an acceleration procedure.)
- $\boldsymbol{N}(f;\boldsymbol{x},\check{x})\subset\boldsymbol{x}$ implies there is a unique solution to $f(x)=0$ in $\boldsymbol{N}(f;\boldsymbol{x},\check{x})$, and hence in $\boldsymbol{x}$.
- Another consequence: $\boldsymbol{N}(f;\boldsymbol{x},\check{x})\cap\boldsymbol{x}=\emptyset$ implies $\boldsymbol{x}$ is fathomed, and $\boldsymbol{x}$ may be discarded.
- Interval Newton methods are locally quadratically convergent.

Outline

GlobSol

A Brief Summary

- It began in 1985 as `INTBIS`, an *ACM Transactions on Mathematical Software* algorithm that implemented a branch-and-bound technique for finding all solutions to polynomial systems.
- With funding from various public and private sources, and with participation of graduate students, GlobSol developed into a software package for more general constrained and unconstrained global optimization and solution of nonlinear systems.
- A series of presentations and papers on GlobSol is available from `http://interval.louisiana.edu/preprints.htm`
- Interval techniques and traditional techniques in optimization are merging, and development is continuing.

GlobSol

A Brief Summary

- It began in 1985 as `INTBIS`, an *ACM Transactions on Mathematical Software* algorithm that implemented a branch-and-bound technique for finding all solutions to polynomial systems.
- With funding from various public and private sources, and with participation of graduate students, GlobSol developed into a software package for more general constrained and unconstrained global optimization and solution of nonlinear systems.
- A series of presentations and papers on GlobSol is available from `http://interval.louisiana.edu/preprints.ht`
- Interval techniques and traditional techniques in optimization are merging, and development is continuing.

GlobSol

A Brief Summary

- It began in 1985 as `INTBIS`, an *ACM Transactions on Mathematical Software* algorithm that implemented a branch-and-bound technique for finding all solutions to polynomial systems.
- With funding from various public and private sources, and with participation of graduate students, GlobSol developed into a software package for more general constrained and unconstrained global optimization and solution of nonlinear systems.
- A series of presentations and papers on GlobSol is available from `http://interval.louisiana.edu/preprints.htr`
- Interval techniques and traditional techniques in optimization are merging, and development is continuing.

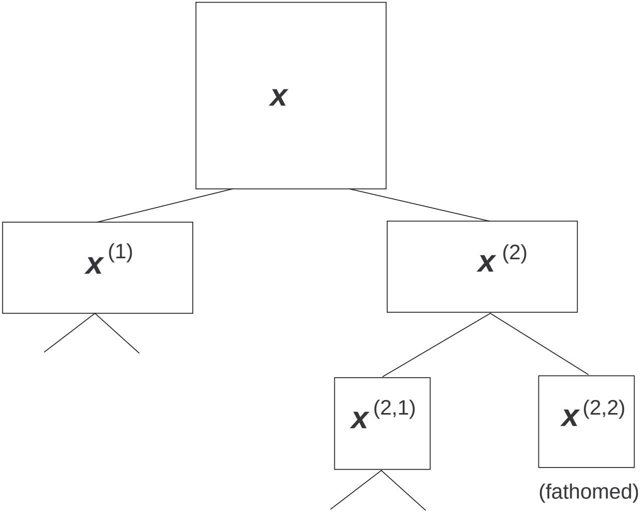
GlobSol

A Brief Summary

- It began in 1985 as `INTBIS`, an *ACM Transactions on Mathematical Software* algorithm that implemented a branch-and-bound technique for finding all solutions to polynomial systems.
- With funding from various public and private sources, and with participation of graduate students, GlobSol developed into a software package for more general constrained and unconstrained global optimization and solution of nonlinear systems.
- A series of presentations and papers on GlobSol is available from `http://interval.louisiana.edu/preprints.htm`
- Interval techniques and traditional techniques in optimization are merging, and development is continuing.

A Box Search Tree

(With intervals,we usually use boxes, not simplices.)



The Degree Has Its Place

- Interval Newton methods do not handle solutions at which the Jacobi matrix (or Kuhn–Tucker matrix) is singular, or where the solution set is not isolated, whereas the topological degree does.
- Singularities and non-isolated solutions seem to be very common in applied optimization problems.
- Degree computation can be incorporated into global optimization algorithms.
- Conversely, interval methods can be incorporated into topological degree algorithms for other applications..

The Degree Has Its Place

- Interval Newton methods do not handle solutions at which the Jacobi matrix (or Kuhn–Tucker matrix) is singular, or where the solution set is not isolated, whereas the topological degree does.
- Singularities and non-isolated solutions seem to be very common in applied optimization problems.
- Degree computation can be incorporated into global optimization algorithms.
- Conversely, interval methods can be incorporated into topological degree algorithms for other applications..

The Degree Has Its Place

- Interval Newton methods do not handle solutions at which the Jacobi matrix (or Kuhn–Tucker matrix) is singular, or where the solution set is not isolated, whereas the topological degree does.
- Singularities and non-isolated solutions seem to be very common in applied optimization problems.
- Degree computation can be incorporated into global optimization algorithms.
- Conversely, interval methods can be incorporated into topological degree algorithms for other applications..

The Degree Has Its Place

- Interval Newton methods do not handle solutions at which the Jacobi matrix (or Kuhn–Tucker matrix) is singular, or where the solution set is not isolated, whereas the topological degree does.
- Singularities and non-isolated solutions seem to be very common in applied optimization problems.
- Degree computation can be incorporated into global optimization algorithms.
- Conversely, interval methods can be incorporated into topological degree algorithms for other applications..

Improvement of the Topological Degree Algorithm

- Oliver Aberth began with Frank's original work, with Kearfott's continuation, to publish an algorithm for computation of the topological degree based on finding all solutions to a system derived from F on $\partial\mathcal{D}$.
- See Oliver Aberth, "Computation of the Topological Degree Using Interval Arithmetic, and Applications," *Math. Comp.* **62**, 205, pp. 171–178 (1994).
- Also see Oliver Aberth, *Introduction to Precise Numerical Methods*, second edition, Academic Press, 2007.

(slide 67)

Improvement of the Topological Degree Algorithm

- Oliver Aberth began with Frank's original work, with Kearfott's continuation, to publish an algorithm for computation of the topological degree based on finding all solutions to a system derived from F on $\partial\mathcal{D}$.
- See Oliver Aberth, "Computation of the Topological Degree Using Interval Arithmetic, and Applications," *Math. Comp.* **62**, 205, pp. 171–178 (1994).
- Also see Oliver Aberth, *Introduction to Precise Numerical Methods*, second edition, Academic Press, 2007.

Improvement of the Topological Degree Algorithm

- Oliver Aberth began with Frank's original work, with Kearfott's continuation, to publish an algorithm for computation of the topological degree based on finding all solutions to a system derived from F on $\partial\mathcal{D}$.
- See Oliver Aberth, "Computation of the Topological Degree Using Interval Arithmetic, and Applications," *Math. Comp.* **62**, 205, pp. 171–178 (1994).
- Also see Oliver Aberth, *Introduction to Precise Numerical Methods*, second edition, Academic Press, 2007.

Alternate Ways of Incorporating the Degree

- Jianwei Dian developed a highly efficient technique for computing the topological index of solutions to $F = 0$ in $\mathbb{R}^n$ and $\mathbb{C}^n$.
  - "Existence Verification of Higher Degree Singular Zeros of Nonlinear Systems," Ph.D. dissertation, University of Louisiana at Lafayette, 2000.
  - J. Dian and R. B. Kearfott, "Existence Verification for Singular and Non-Smooth Zeros of Real Nonlinear Systems," *Math. Comp.* **72**, 242, pp. 757–766 (2003).
  - R. B. Kearfott, J. Dian, and A. Neumaier, "Existence Verification for Singular Zeros of Complex Nonlinear Systems," *SIAM J. Numer. Anal.* **38**, 2, pp. 360–379 (2000).
- More can be done along these lines, both in theory and in practice.

Alternate Ways of Incorporating the Degree

- Jianwei Dian developed a highly efficient technique for computing the topological index of solutions to $F = 0$ in $\mathbb{R}^n$ and $\mathbb{C}^n$.
  - "Existence Verification of Higher Degree Singular Zeros of Nonlinear Systems," Ph.D. dissertation, University of Louisiana at Lafayette, 2000.
  - J. Dian and R. B. Kearfott, "Existence Verification for Singular and Non-Smooth Zeros of Real Nonlinear Systems," *Math. Comp.* **72**, 242, pp. 757–766 (2003).
  - R. B. Kearfott, J. Dian, and A. Neumaier, "Existence Verification for Singular Zeros of Complex Nonlinear Systems," *SIAM J. Numer. Anal.* **38**, 2, pp. 360–379 (2000).
- More can be done along these lines, both in theory and in practice.

Alternate Ways of Incorporating the Degree

- Jianwei Dian developed a highly efficient technique for computing the topological index of solutions to $F = 0$ in $\mathbb{R}^n$ and $\mathbb{C}^n$.
  - "Existence Verification of Higher Degree Singular Zeros of Nonlinear Systems," Ph.D. dissertation, University of Louisiana at Lafayette, 2000.
  - J. Dian and R. B. Kearfott, "Existence Verification for Singular and Non-Smooth Zeros of Real Nonlinear Systems," *Math. Comp.* **72**, 242, pp. 757–766 (2003).
  - R. B. Kearfott, J. Dian, and A. Neumaier, "Existence Verification for Singular Zeros of Complex Nonlinear Systems," *SIAM J. Numer. Anal.* **38**, 2, pp. 360–379 (2000).
- More can be done along these lines, both in theory and in practice.

Alternate Ways of Incorporating the Degree

- Jianwei Dian developed a highly efficient technique for computing the topological index of solutions to $F = 0$ in $\mathbb{R}^n$ and $\mathbb{C}^n$.
  - "Existence Verification of Higher Degree Singular Zeros of Nonlinear Systems," Ph.D. dissertation, University of Louisiana at Lafayette, 2000.
  - J. Dian and R. B. Kearfott, "Existence Verification for Singular and Non-Smooth Zeros of Real Nonlinear Systems," *Math. Comp.* **72**, 242, pp. 757–766 (2003).
  - R. B. Kearfott, J. Dian, and A. Neumaier, "Existence Verification for Singular Zeros of Complex Nonlinear Systems," *SIAM J. Numer. Anal.* **38**, 2, pp. 360–379 (2000).
- More can be done along these lines, both in theory and in practice.

Alternate Ways of Incorporating the Degree

- Jianwei Dian developed a highly efficient technique for computing the topological index of solutions to $F = 0$ in $\mathbb{R}^n$ and $\mathbb{C}^n$.
  - "Existence Verification of Higher Degree Singular Zeros of Nonlinear Systems," Ph.D. dissertation, University of Louisiana at Lafayette, 2000.
  - J. Dian and R. B. Kearfott, "Existence Verification for Singular and Non-Smooth Zeros of Real Nonlinear Systems," *Math. Comp.* **72**, 242, pp. 757–766 (2003).
  - R. B. Kearfott, J. Dian, and A. Neumaier, "Existence Verification for Singular Zeros of Complex Nonlinear Systems," *SIAM J. Numer. Anal.* **38**, 2, pp. 360–379 (2000).
- More can be done along these lines, both in theory and in practice.