Validation for scientific computations Interval arithmetic

Cours de recherche master informatique

Nathalie Revol

Nathalie.Revol@ens-lyon.fr

26 January 2007

References for today's lecture

- R. Moore: *Interval Analysis*, Prentice Hall, Englewood Cliffs, 1966.
- A. Neumaier: Interval methods for systems of equations, CUP, 1990.
- E. Hansen and W. Walster: *Global optimization using interval analysis*, MIT Press, 2004.
- R.B. Kearfott: *Rigorous global search: continuous problems*, Kluwer, 1996.
- V. Kreinovich, A. Lakeyev, J. Rohn, P. Kahl: *Computational Complexity and Feasibility of Data Processing and Interval Computations*, Dordrecht, 1997.
- L.H. Figueiredo, J. Stolfi: *Affine arithmetic* http://www.ic. unicamp.br/~stolfi/EXPORT/projects/affine-arith/.
- *Taylor models arith.:* M. Berz and K. Makino, N. Nedialkov, M. Neher.

Historical remarks

Who invented Interval Arithmetic?

- Ramon Moore in 1962 1966 ?
- T. Sunaga in 1958 ?
- Rosalind Cecil Young in 1931 ?

Cf. http://www.cs.utep.edu/interval-comp/, click on *Early papers*.

Popularization in the 1980, German school (U. Kulisch).

IEEE-754 standard for floating-point arithmetic in 1985: directed roundings are standardized and available (?).

Since the nineties: interval algorithms.

A brief introduction

Interval arithmetic: replace numbers by intervals and compute.

Fundamental theorem of interval arithmetic:

(or "Thou shalt not lie"):

the exact result (number or set) is contained in the computed interval.

No result is lost, the computed interval is guaranteed to contain every possible result.

A brief introduction

Interval Arithmetic and validated scientific computing: two directions

- 1. replace floating-point arithmetic by interval arithmetic to bound from above roundoff errors;
- 2. replace floating-point arithmetic and algorithms by interval ones to compute guaranteed enclosures.

A brief introduction

Interval arithmetic: replace numbers by intervals and compute.

Initially: introduced to take into account roundoff errors (Moore 1966) and also uncertainties (on the physical data...). Then: computations "in the large", computations with sets.

Interval analysis: develop algorithms for **reliable (or verified, or guaranteed) computing**,

that are suited for interval arithmetic,

i.e. different from the algorithms from classical numerical analysis.

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A brief introduction: examples of applications

- control the roundoff errors, cf. computational geometry
- solve several problems with verified solutions: linear and nonlinear systems of equations and inequations, constraints satisfaction, (non/convex, un/constrained) global optimization, integrate ODEs e.g. particules trajectories. . .
- mathematical proofs: cf. Hales' proof of the Kepler's conjecture

Cf. http://www.cs.utep.edu/interval-comp/

Agenda

- Definitions of interval arithmetic (operations, function extensions)
- Cons (overestimation, complexity) and pros (contractant iterations: Brouwer's theorem)
- Some algorithms
 - solving linear systems
 - Newton
 - global optimization wo/with constraints
 - constraints programming
- Variants: affine arithmetic, Taylor models arithmetic

Agenda

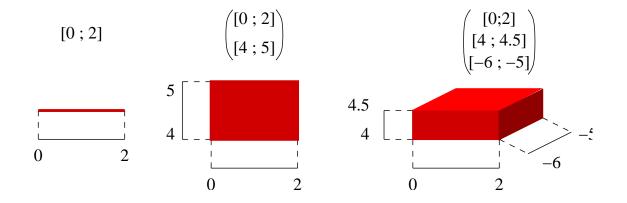
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Definitions: intervals

Objects:

• intervals of real numbers = closed connected sets of ${\mathbb R}$

- interval for π : [3.14159, 3.14160]
- data d measured with an absolute error less than $\pm \varepsilon$: $[d \varepsilon, d + \varepsilon]$
- interval vector: components = intervals; also called box



• interval matrix: components = intervals.

Definitions: operations

 $x \diamond y = Hull \{x \diamond y : x \in x, y \in y\}$ Arithmetic and algebraic operations: use the monotony

Definitions: operations

Algebraic properties: associativity, commutativity hold, some are lost:

- subtraction is not the inverse of addition, in particular $m{x} m{x}
 eq [0]$
- division is not the inverse of multiplication
- squaring is tighter than multiplication by oneself
- multiplication is only sub-distributive wrt addition

Definitions: functions

Definition:

an interval extension f of a function f satisfies

$$\forall \boldsymbol{x}, \ f(\boldsymbol{x}) \subset \boldsymbol{f}(\boldsymbol{x}), \ \text{and} \ \forall x, \ f(\{x\}) = \boldsymbol{f}(\{x\}).$$

Elementary functions: again, use the monotony.

$$\exp \boldsymbol{x} = [\exp \underline{x}, \exp \overline{x}]$$

$$\log \boldsymbol{x} = [\log \underline{x}, \log \overline{x}] \text{ if } \underline{x} \ge 0, [-\infty, \log \overline{x}] \text{ if } \overline{x} > 0$$

$$\sin[\pi/6, 2\pi/3] = [1/2, 1]$$

...

Definitions: function extension

Example: $f(x) = x^2 - x + 1$ with $x \in [-2, 1]$.

$$\begin{split} & [-2,1]^2 - [-2,1] + 1 = [0,4] + [-1,2] + 1 = [0,7].\\ & \text{Since } x^2 - x + 1 = x(x-1) + 1, \text{ we get } [-2,1] \cdot ([-2,1]-1) + 1 = \\ & [-2,1] \cdot [-3,0] + 1 = [-3,6] + 1 = [-2,7].\\ & \text{Since } x^2 - x + 1 = (x-1/2)^2 + 3/4, \text{ we get } ([-2,1]-1/2)^2 + 3/4 = \\ & [-5/2,1/2]^2 + 3/4 = [0,25/4] + 3/4 = [3/4,7] = f([-2,1]). \end{split}$$

Problem with this definition: infinitely many interval extensions, syntactic use (instead of semantic).
How to choose the best extension? How to choose a good one?

Definitions: function extension

Mean value theorem of order 1 (Taylor expansion of order 1): $\forall x, \forall y, \exists \xi_{x,y} \in (x, y) : f(y) = f(x) + (y - x) \cdot f'(\xi_{x,y})$ Interval interpretation:

$$\forall y \in \boldsymbol{x}, \forall \tilde{x} \in \boldsymbol{x}, \ f(y) \in f(\tilde{x}) + (y - \tilde{x}) \cdot \boldsymbol{f}'(\boldsymbol{x}) \\ \Rightarrow f(\boldsymbol{x}) \subset f(\tilde{x}) + (\boldsymbol{x} - \tilde{x}) \cdot \boldsymbol{f}'(\boldsymbol{x})$$

Mean value theorem of order 2 (Taylor expansion of order 2): $\forall x, \forall y, \exists \xi_{x,y} \in (x,y) : f(y) = f(x) + (y-x) \cdot f'(x) + \frac{(y-x)^2}{2} \cdot f''(\xi_{x,y})$ Interval interpretation:

$$\forall y \in \boldsymbol{x}, \forall \tilde{x} \in \boldsymbol{x}, f(y) \in f(\tilde{x}) + (y - \tilde{x}) \cdot f'(\tilde{x}) + \frac{(y - \tilde{x})^2}{2} \cdot \boldsymbol{f}''(\boldsymbol{x}) \\ \Rightarrow f(\boldsymbol{x}) \subset f(\tilde{x}) + (\boldsymbol{x} - \tilde{x}) \cdot f'(\tilde{x}) + \frac{(x - \tilde{x})^2}{2} \cdot \boldsymbol{f}''(\boldsymbol{x})$$

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Definitions: function extension No need to go further:

- it is difficult to compute (automatically) the derivatives of higher order, especially for multivariate functions;
- there is no (theoretical) gain in quality.

Theorem:

- for the natural extension ${\pmb f}$ of f, it holds $d(f({\pmb x}), {\pmb f}({\pmb x})) \leq \mathcal{O}(w({\pmb x}))$
- for the first order Taylor extension f_{T_1} of f, it holds $d(f(x), f_{T_1}(x)) \le O(w(x)^2)$
- getting an order higher than 3 is impossible without the squaring operation, is difficult even with it...

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Cons: overestimation (1/2)

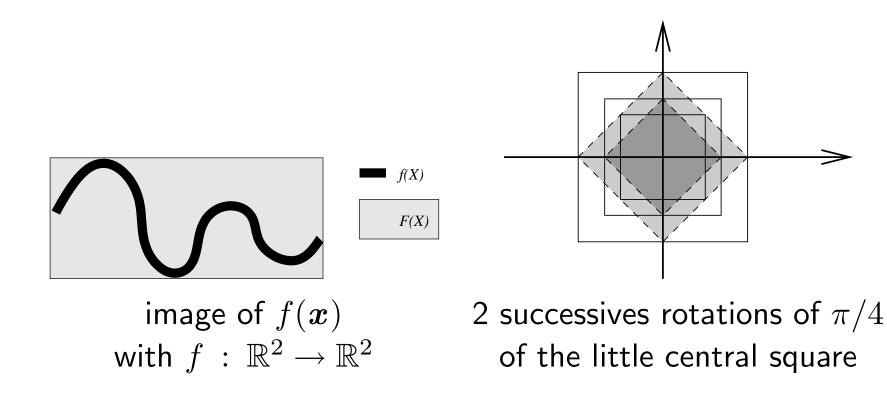
The result encloses the true result, but it is too large: overestimation phenomenon. Two main sources: variable dependency and wrapping effect.

(Loss of) Variable dependency:

$$x - x = \{x - y : x \in x, y \in x\} \neq \{x - x : x \in x\} = \{0\}.$$

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Cons: overestimation (2/2)



Cons: Complexity: almost every problem is NP-hard

Gaganov 1982, Rohn 1994 ff, Kreinovich. . .

- evaluate a function on a box (cartesian product of intervals)
- evaluate a function on a box up to ε
- solve a linear system
- solve a linear system up to $1/4n^4$ ($n = \dim$ of the system)
- determine if the solution of a linear system is bounded
- compute the matrix norm $\|oldsymbol{A}\|_{\infty,1}$
- determine if an interval matrix (= a matrix with interval coefficients) is regular, i.e. if every possible punctual matrix in it is regular

Cons: Complexity: Gaganov 1982

evaluation of a multivariate polynomial with rational coeff. on a box is NP-hard

Idea: reduce polynomially the CNF-3 problem to this problem. On n boolean variables q_1, \dots, q_n , a formula f in CNF-3 is defined by

$$f = \bigwedge_{i=1}^{m} f_i \text{ with } f_i = \bigvee_{j=1}^{1,2or3} r_{i,j}$$

with $r_{i,j} = q_{k_{i,j}}$ or $r_{i,j} = \neg q_{k_{i,j}}$.

1. to each boolean variable q_i , let us associate a real variable $x_i \in [0, 1]$. Meaning: $x_i = 0$ if $q_i = F$ and $x_i = 1$ if $q_i = T$.

- * Goal: get a polynomial which takes only values in [0, 1]i.e. allow only product of terms or sums of the form (1- term). A product corresponds to a conjunction and 1-x to a negation \Rightarrow express f and the f_i using conjonctions and negations \Rightarrow express the f_i as $\neg \bigwedge_{i=1}^{1,2or3} \neg r_{i,j}$.
- 2. to each $r_{i,j}$ let us associate a polynomial $y_{i,j}$ (corresponding to the negation of $r_{i,j}$) defined by

3. to each f_i , let us associate a polynomial p_i (corresponding to the negation of f_i) defined by $f_i = \bigwedge r_{i,j} \rightarrow p_i(x) = \prod y_{i,j}(x)$.

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4. to f, let us associate the polynomial p defined by $f = \bigwedge_{i=1}^{m} f_i \rightarrow p(x) = \prod_{i=1}^{m} (1 - p_i(x)).$

Cons: Complexity: Gaganov 1982

evaluation of a multivariate polynomial with rational coeff. on a box is NP-hard

Lemma:

1. $\forall x \in [0, 1], p(x) \in [0, 1].$

2. if α is a boolean vector and β is the associated 0-1 vector, then

$$f(\alpha) = T \Rightarrow p(\beta) = 1$$

$$f(\alpha) = F \Rightarrow p(\beta) = 0.$$

3. if f is not feasible, then $\forall x \in [0,1]^n$, $p(x) \leq 7/8$.

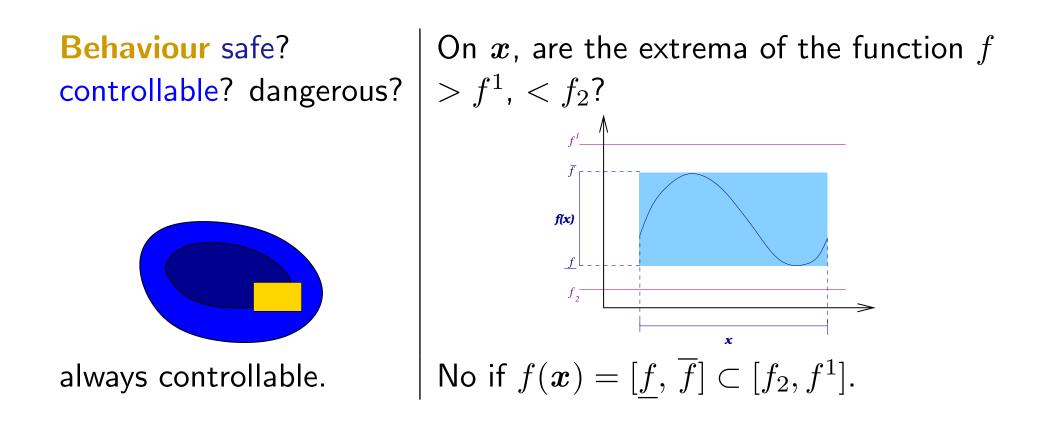
Proof of (3): (proving (1) and (2) is easy).

 $\forall x \in [0,1]^n$, let us consider β the 0-1 vector obtained by rounding x to the nearest.

Since f is not feasible, $p(\beta) = 0$. Since $p(x) = \prod_{i=1}^{m} (1 - p_i(x))$, $\exists i_0$ such that $1 - p_{i_0}(\beta) = 0$. One can prove that $p_{i_0}(x) \ge 1/8$, using the fact that it is the product of at most three terms, each of them $\le 1/2$, using the fact that β is the rounding to nearest of x. Thus $1 - p_{i_0}(x) \le 7/8$. The remaining factors $1 - p_j(x)$ are less or equal to 1. Thus $p(x) = \prod_{i=1}^{m} (1 - p_i(x)) \le 7/8$.

Consequence: since checking the feasibility of a CNF-3 formula is NP-hard, evaluating a multivariate polynomial (up to a small ε) is NP-hard.

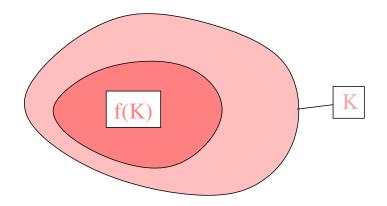
Pros: set computing



Pros: Brouwer-Schauder theorem

A function f which is continuous on the unit ball B and which satisfies $f(B) \subset B$ has a fixed point on B.

Furthermore, if $f(B) \subset intB$ then f has a unique fixed point on B.



The theorem remains valid if B is replaced by a box K.

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Algorithm: linear systems solving (Hansen-Sengupta) Problem: solve Ax = b or equivalently:

$$oldsymbol{A}_{i,1}oldsymbol{x}_1+\ldots+oldsymbol{A}_{i,n}oldsymbol{x}_n=oldsymbol{b}_i$$
 for $1\leq i\leq n$

Determine Hull $(\Sigma_{\exists\exists}(A, b)) = Hull (\{x : \exists A \in A, \exists b \in b, Ax = b\}).$

Pre-processing: multiply the system by an approximate $mid(\mathbf{A})^{-1}$. New system $= mid(\mathbf{A})^{-1}\mathbf{A}\mathbf{x} = \mathbf{b}$. Hope: contracting iteration.

Algorithm: apply Gauss-Seidel iteration while convergence not reached loop for i = 1 to n do $x_i := \left(b_i - \sum_{j \neq i} A_{i,j} x_j \right) / A_{i,i}$

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Algorithm: solving a nonlinear system: Newton Why a specific iteration for interval computations?

Usual formula:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

Direct interval transposition:

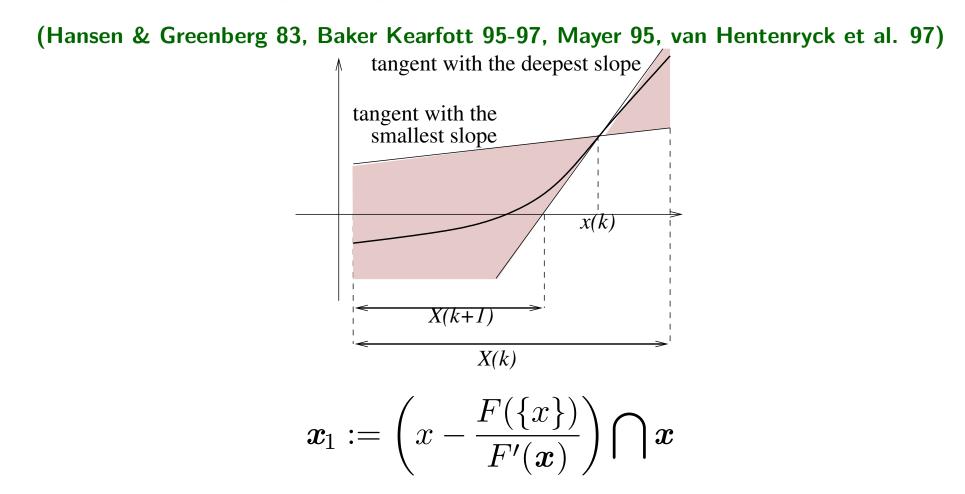
$$oldsymbol{x}_{k+1} = oldsymbol{x}_k - rac{f(oldsymbol{x}_k)}{f'(oldsymbol{x}_k)}$$

$$w(\boldsymbol{x}_{k+1}) = w(\boldsymbol{x}_k) + w\left(\frac{f(\boldsymbol{x}_k)}{f'(\boldsymbol{x}_k)}\right) > w(\boldsymbol{x}_k)$$

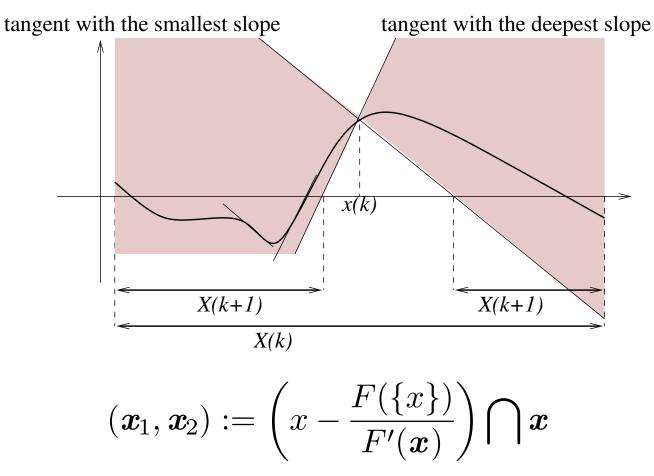
divergence!

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Algorithm: interval Newton principle of an iteration



Algorithm: interval Newton principle of an iteration



Algorithm: interval Newton

Input: F, F', $x_0 = //x_0$ initial search interval **Initialization:** $\mathcal{L} = \{x_0\}, \alpha = 0.75$ //any value in]0.5, 1[is suitable **Loop:** while $\mathcal{L} \neq \emptyset$ Suppress $(\boldsymbol{x}, \mathcal{L})$ $x := \operatorname{mid}(\boldsymbol{x})$ $(x_1, x_2) := \left(x - rac{F(\{x\})}{F'(x)}
ight) \cap x$ // x_1 and x_2 can be empty if $w(\boldsymbol{x}_1) > \alpha w(\boldsymbol{x})$ or $w(\boldsymbol{x}_2) > \alpha w(\boldsymbol{x})$ then $(\boldsymbol{x}_1, \boldsymbol{x}_2) := \mathsf{bisect}(\boldsymbol{x})$ if $\boldsymbol{x}_1 \neq \emptyset$ and $F(\boldsymbol{x}_1) \ni 0$ then if $w(x_1)/|\operatorname{mid}(x_1)| \leq \varepsilon_x$ or $w(F(x_1)) \leq \varepsilon_Y$ then Insert x_1 in Res else Insert x_1 in \mathcal{L} same handling of x_2

Output: *Res*, a list of intervals that may contain the roots.

Algorithm: interval Newton

Existence and uniqueness of a root are proven:

if there is no hole and if the new iterate (before \bigcap) is contained in the interior of the previous one.

Existence of a root is proven:

- using the mean value theorem:
 OK if f(inf(x)) and f(sup(x)) have opposite signs.
 (Miranda theorem in higher dimensions).
- using Schauder theorem: if the new iterate (before ∩) in contained in the previous one.

Algorithm: optimize a continuous function

Problem: $f : \mathbb{R}^n \to \mathbb{R}$, determine x^* and f^* that verify

$$f^* = f(x^*) = \min_x f(x)$$

Assumptions:

- search within a box x_0
- $x^* \in$ in the interior of (x_0) , not at the boundary
- f continuous enough: \mathcal{C}^2

Algorithm: optimize a continuous function

(Ratschek and Rokne 1988, Hansen 1992, Kearfott 1996...)

Goal: determine the minimum of f, continuous function on a box x_0 .

 x_0 current box

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\bar{f} current upper bound of f^{\ast}
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while there is a box in the waiting list

if f(x) > \overline{f} then

reject x

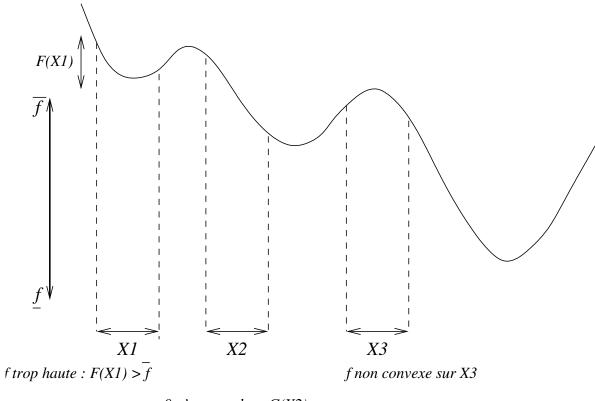
otherwise

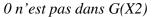
update \overline{f}: if f(mid(x)) < \overline{f} then \overline{f} = f(mid(x))

bisect x into x_1 and x_2

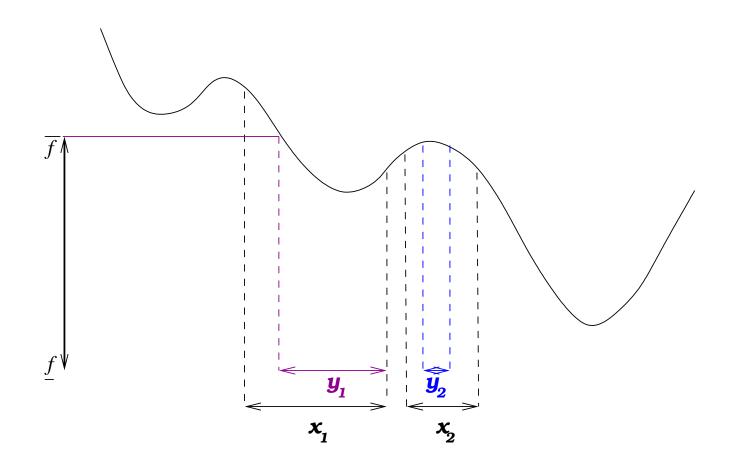
examine x_1 and x_2
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Algorithm: optimize a continuous function the rejection procedure





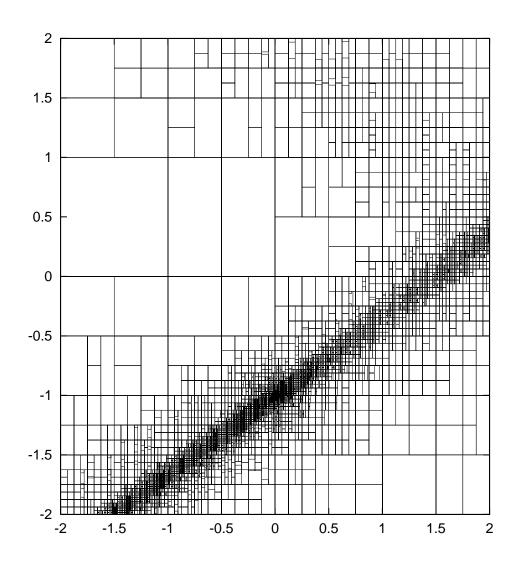
Algorithm: optimize a continuous function the reduction procedure



Algorithm: optimize a continuous function

Hansen algorithm Hansen 1992

 $\mathcal{L} =$ list of not yet examined boxes := { x_0 } while $\mathcal{L} \neq \emptyset$ loop remove x from \mathcal{L} reject x? yes if $f(\boldsymbol{x}) > \bar{f}$ ves if $\operatorname{Grad} f(\boldsymbol{x}) \not\supseteq 0$ yes if $Hf(\boldsymbol{x})$ has its diagonal non > 0reduce xNewton applied to the gradient solve $\boldsymbol{y} \subset \boldsymbol{x}$ such that $f(\boldsymbol{y}) \leq \overline{f}$ **bisect** y: insert the resulting y_1 and y_2 in \mathcal{L}



Algorithm: constrained optimization

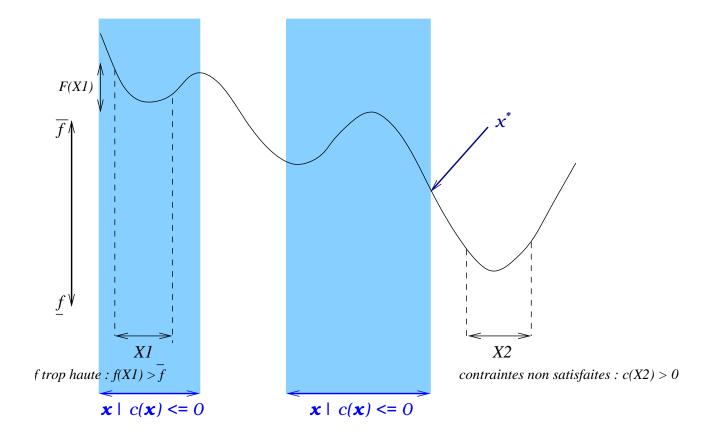
Problem: $f : \mathbb{R}^n \to \mathbb{R}$ and $c : \mathbb{R}^n \to \mathbb{R}^m$, determine x^* and f^* that verify

$$f^* = f(x^*) = \min_{\{x \mid c(x) \le 0\}} f(x)$$

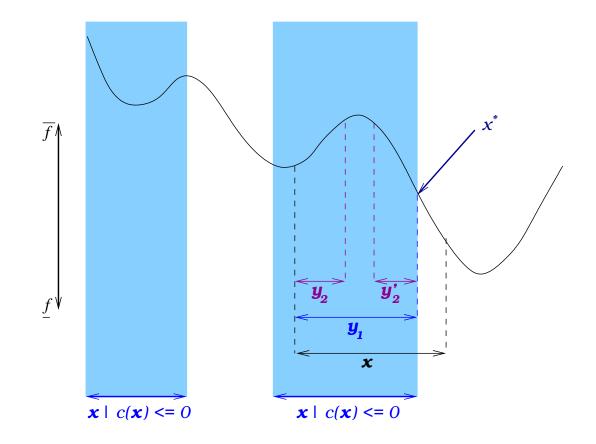
Assumptions:

- search within a box x_0
- f continuous enough: \mathcal{C}^2
- c continuous enough: \mathcal{C}^1

Algorithm: constrained optimization $c(x) \le 0$ the rejection procedure



Algorithm: constrained optimization $c(x) \le 0$ the reduction procedure



Algorithm: constrained optimization $c(\mathbf{x}) \leq 0$ $\mathcal{L} := \{ \boldsymbol{x}_0 \}$ $\mathcal{L} := \{x_0\}$ while $\mathcal{L} \neq \emptyset$ loop while $\mathcal{L} \neq \emptyset$ loop remove x from $\mathcal L$ remove x from $\mathcal L$ reject x? reject x? yes if $f(\boldsymbol{x}) > \overline{f}$ yes if $f(\boldsymbol{x}) > f$ yes if $c(\boldsymbol{x}) > 0$ yes if $\operatorname{Grad} f(\boldsymbol{x}) \not\ni 0$ yes if f not convex on xreduce xreduce xsolve $\boldsymbol{y} \subset \boldsymbol{x} \mid f(\boldsymbol{y}) \leq \bar{f}$ 'solve $\boldsymbol{y} \subset \boldsymbol{x}$ such that $c(\boldsymbol{y}) \leq$ Newton applied to the gradient Newton applied to the Lagran **bisect** y into y_1 and y_2 **bisect** \boldsymbol{y} into \boldsymbol{y}_1 and \boldsymbol{y}_2 insert $oldsymbol{y}_1$ and $oldsymbol{y}_2$ in $\mathcal L$ insert $oldsymbol{y}_1$ and $oldsymbol{y}_2$ in $\mathcal L$

Algorithm: constraints programming

Cleary 1987, Benhamou et al. 1999, Jaulin et al. 2001

Problem:

$$\begin{cases} c_1(x_1,\ldots,x_n) = 0 \\ \vdots \\ c_p(x_1,\ldots,x_n) = 0 \end{cases}$$

expressed as:

$$\begin{array}{rcl}y_i &=& x_i & \mbox{ for } 1 \leq i \leq n \\ y_k &=& y_i \diamond y_j & \mbox{ for } n+1 \leq k \leq m \mbox{ and } i,j < k \\ & y_k \mbox{ auxiliary variable} \\ \mbox{where} & y_k &=& \varphi(y_i) & \mbox{ for } n+1 \leq k \leq m \mbox{ and } i < k \end{array}$$

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Algorithm: constraints programming

Initializations: $oldsymbol{y}_1 := oldsymbol{x}_1, \dots, oldsymbol{y}_n := oldsymbol{x}_n$

Propagation: forward mode

for k = n + 1 to m loop $oldsymbol{y}_k := oldsymbol{y}_i \diamond oldsymbol{y}_j$ or $oldsymbol{y}_k := arphi(oldsymbol{y}_i)$

Propagation: backward mode

for k = m to n loop if y_k is defined as $y_i \diamond y_j$ then $y_i := (y_k \diamond^{-r} y_j) \cap y_i$ $y_j := (y_i \diamond^{-l} y_k) \cap y_j$ else if y_k is defined as $\varphi(y_i)$ then $y_i := \varphi^{-1}(y_k) \cap y_i$ Algorithm: constraints programming: {

$$\begin{cases} x_1 x_2^2 - 2x_3 = 0\\ \cos x_1 + x_3 = 0 \end{cases}$$

Algorithm: constraints programming: {

$$\begin{cases} x_1 x_2^2 - 2x_3 = 0\\ \cos x_1 + x_3 = 0 \end{cases}$$

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Problem:
$$\begin{cases} x_1 x_2^2 - 2x_3 = 0\\ \cos x_1 + x_3 = 0 \end{cases}$$

with
$$x_1 = [0, \frac{2\pi}{3}]$$
, $x_2 = [-1, 1]$, $x_3 = [-\frac{1}{2}, 3]$.

Optimal solution obtained after two iterations:
$$x_1 = [\frac{\pi}{2}, \frac{2\pi}{3}]$$
, $x_2 = [-\sqrt{\frac{2}{\pi}}, \sqrt{\frac{2}{\pi}}]$, $x_3 = [0, \frac{1}{2}]$.

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Conclusions

Interval algorithms

- can solve problems that other techniques are not able to solve
- is a simple version of set computing
- give effective versions of theorems which did not seem to be effective (Brouwer)
- can determine all zeros or all extrema of a continuous function
- overestimate the result
- is less efficient than floating-point arithmetic (theoretical factor: 4, practical factor: 20)
 - \Rightarrow solve "small" problems.

Philosophical conclusion

Morale

- forget one's biases:
 - do not use without thinking algorithms which are supposed to be good ones (Newton)
 - do not reject without thinking algorithm which are supposed to be bad ones (Gauss-Seidel)
- prefer contracting iterations whenever possible