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OPTIMIZATION USING INTERVAL MATHEMATICS

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Abstract

The paper gives a summary of the tools and methods of Interval Mathematics which can be used in optimization. The purpose is to get exact and narrow bounds for both the optimal value aund for the location where it will be reached. Interval methods and algorithms are discussed including interval decision criteria for accepting or rejecting subsets.

1. The original problem

Given are: The dimension $n \in \mathbb{N}$,

the basic set $B \subseteq \mathbb{R}^n$,

the mapping $f : B \to \mathbb{R}$.

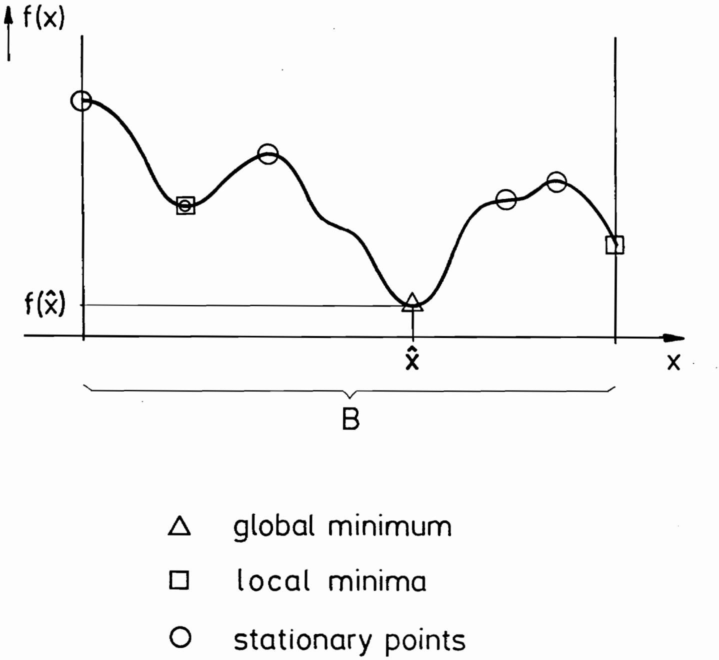
Wanted are

i) $\hat{x} \in B$ such that $f(\hat{x}) = \min_{x \in B} f(x)$;

ii) $y := f(\hat{x})$.

See Figure 1.

AMS Subject Classifications: 65K10, 65G10



<u>Figure 1</u>. The original problem for n = 1.

The following result is well known:

<u>Theorem</u>: Let B be compact and let f be continuous on B. Then $\exists\, \hat{x} \in B$.

<u>Remarks</u>: 1) In general $\hat{x}$ is <u>not</u> unique.

2) The above cited problem is normally called "unconstrained", even if $B \neq \mathbb{R}^n$ ("bound constraint").

3) By replacing f by -f the above "minimizing" problem is changed to a "maximizing" problem.

The main problem of optimization is not the existence problem but the problem:

HOW TO FIND $\hat{X}$?
HOW TO FIND $Y := F(\hat{X})$?

In what follows for simplicity the following assumptions are made:

i) The basic set $B \subseteq \mathbb{R}^n$ is a box (i.e. an n-dimensional interval).

ii) The function f is sufficiently smooth. All derivatives f' and f" do exist whenever they are mentioned.

iii) All the figures are drawn for the simplest case $n = 1$.

There are two general classes of methods for solving numerically the above problem:

i) descend methods;

ii) methods for solving $f'(x) = 0$ (i.e. search for stationary points).

Both will subsequently be discussed.

In Numerical Analysis two different approaches for tackling numerically a problem are possible:

I (Theoretical) Methods: Infinitely many steps are permitted; numbers are regarded as "exact"; functions are arbitrary; error estimates are given.

II (Numerical) Algorithms: The computer implementation is essential; stop after a finite number of steps (stopping criterium?); rounding of numbers is permitted; only "computable" functions are treated; strict error bounds are looked for.

In the following paper mainly the algorithmic aspect is treated.

2. Practical difficulties

From now on let $f : B \to \mathbb{R}$ be a "computable" function. This is a function generated by a program on a computer. Hence it is piecewise rational.

Theorem. An algorithmic solution of the original problem is in general

impossible !

Reasons: 1) Infinitely many optimal points $\hat{x}$ may exist.

2) Infinitely many steps may be necessary (e.g.: $\hat{x} = \sqrt{2}$).

3) Round off errors, data errors may perturb the problem.

The "best possible" solution may be a "good" approximation $\tilde{x}$ to $\hat{x}$ and $\tilde{y}$ to y such that the distances $\|\hat{x} - \tilde{x}\|$ and $|\tilde{y} - y|$ are "small". This leads to:

3. The Interval Problem

Given are as above: $n \in \mathbb{N}$, $B = [\underline{b}, \overline{b}] \subseteq \mathbb{R}$ and a computable function $f : B \to \mathbb{R}$.

Wanted is an algorithm which produces the following intervals

i) $\hat{X} = [\underline{\hat{x}}, \overline{\hat{x}}] \subseteq B$ with $\hat{x} \in \hat{X}$;

ii) $Y = [\underline{y}, \overline{y}] \subseteq \mathbb{R}$ with $f(\hat{x}) \in Y$,

such that

iii) $\hat{X}$ and Y are "small" and "convergent".

For i) and ii) see Figure 2.

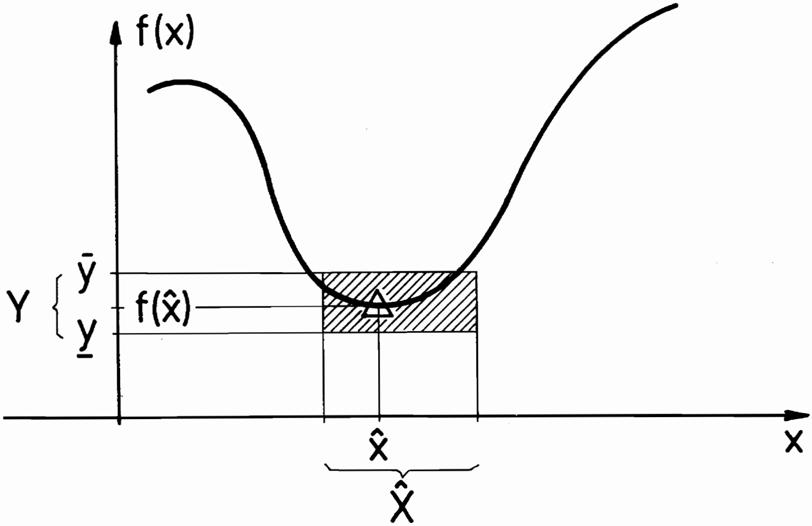


Figure 2: Explanation of the Interval Problem (for n = 1).

4. Interval Mathematics

is a new tool which can be used in addition to known methods.

INTERVAL MATHEMATICS USES SETS (INTERVALS) INSTEAD OF POINTS.

See the list of References. In the first part A) of this list general papers, proceedings and books are listed which may serve as an introduction to this topic. The second part B) contains such interval papers which deal with the computation of the range of a function. (This is more general than optimization).

In the third and final part C) all those papers have been quoted which treat the defined Interval Problem and which are known to the author.

Notations: Define $\mathbb{I}(B)$ as the set of all compact intervals in B and likewise $\mathbb{I}(\mathbb{R}^n)$ and $\mathbb{I}(\mathbb{R}^{n\times n})$ as the sets of all interval n-vectors and n×n-matrices.

Definition: The interval function $F : \mathbb{I}(B) \subseteq \mathbb{I}(\mathbb{R}^n) \to \mathbb{I}(\mathbb{R})$ is called interval extension of the function $f : B \to \mathbb{R}$ on B if:

i) $f(x) \in F(X)$ for all $x \in X \subseteq B$ and

ii) $f(x) = F([x,x])$ for all $x \in X \subseteq B$.

Property: Any interval extension F gives bounds for the range $F^*(X) := \{f(x) \mid x \in X\}$ of $f(x)$ for any interval $X \subseteq B$. See Figure 3.

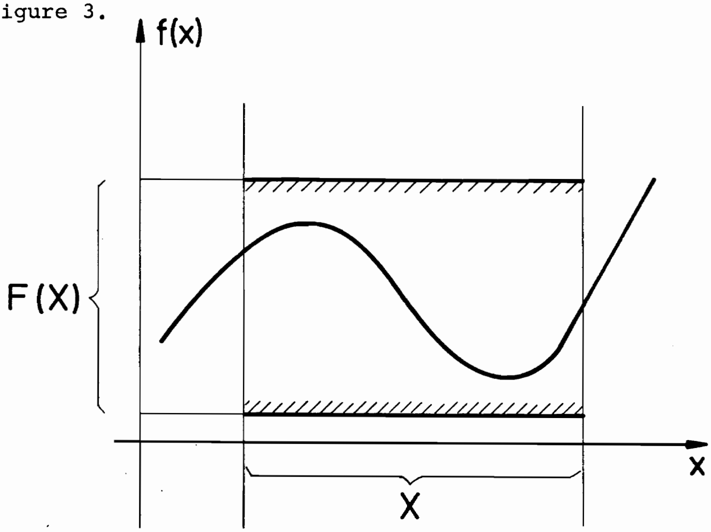


Figure 3. Interval extension F of f on X.

5. Point functions f vs. interval functions F

Any computable function $f : B \to \mathbb{R}$ is

i) piecewise rational, i.e.

ii) piecewise analytic, i.e.

iii) $f, f' f'', \ldots$ can all be evaluated for any $x \in B$ by <u>automatic</u> differentiation (no symbolic differentiation, no numerical approximation), see the book of L.B. Rall (1980).

To any such function f there is a <u>natural</u> interval extension $F : \mathbb{I}(B) \to \mathbb{I}(\mathbb{R})$ (at least for "small" interval arguments $X \subseteq B$). This can also <u>automatically</u> be generated on a computer together with further extensions D, H for the derivatives f', f" such that

$$f \in F, \quad f' \in D, \quad f'' \in H.$$

See again the book of L.B. Rall (1980).

With a computable point function f the above defined optimization problem can not be solved. The reason for this is:

POINT FUNCTIONS GIVE ONLY LOCAL INFORMATION.

Hence f is "known" at most at the finitely many machine numbers. In between these points the behaviour of f is unknown.

(Trivial) Example: Let $n = 1$ and $B := [0,1]$.

Define $f(x) := 0$ for all $x \in B$. There is no imaginable algorithm which can compute that

$$f(\hat{x}) = \min \quad \text{for all } \hat{x} \in [0,1].$$

Opposite to the behaviour of a point function the following is true:

INTERVAL FUNCTIONS GIVE GLOBAL INFORMATION.

Hence $f(x) \in F(X)$ is between known bounds for all (infinitely many) points $x \in X \subseteq B$.

(Trivial) Example: Let $n = 1$ and $B := [0,1]$.

Define $f(x) := 0$ and use the (trivial) interval extension $F(X) := [0,0]$ for $X \subseteq B$. This gives immediately the bounds $\hat{x} \in B$ and $f(\hat{x}) \in F(B) = [0,0]$, hence $f(\hat{x}) \equiv 0$ for all $\hat{x} \in B$.

There is, however, a price to be paid for that property: The range F^* of a function f is in general vastly overestimated by the natural interval extension F. But, if F is Lipschitz continuous, then this overestimation is at most linear, i.e.

$$(*) \qquad |F(X), F^*(X)| = O(\text{span}(X)) \quad \text{for } X \subseteq B.$$

This result is due to R.E. Moore A) (1966). For the definition $|.,.|$ of the distance and span (.) of the width of intervals see the literature (e.g. Ratschek-Rokne A) (1984)).

6. Tools for solving the Interval Problem

6.1 Only f is available

Here no interval method is possible. But an upper bound $\overline{y} \geq f(\hat{x})$ can easily be determined be evaluating $\overline{y} := f(x_0)$ for any $x_0 \in B$. Hence:

Result: $\hat{x} \in B$ is the best possible inclusion.

$f(\hat{x}) \leq \overline{y} := f(x_0)$ for any $x_0 \in B$; no lower bound $\underline{y} \leq f(\hat{x})$ can be found.

6.2 Both f and F are known

Because of $f(x) \in F(X)$ for any $x \in X \subseteq B$ one gets immediately the

a priori bounds $f(\hat{x}) \in Y := F(B)$.

Let $x_0 \in B$ and $X_0 \subseteq B$ and assume $F(X_0) > f(x_0)$, see Figure 4.

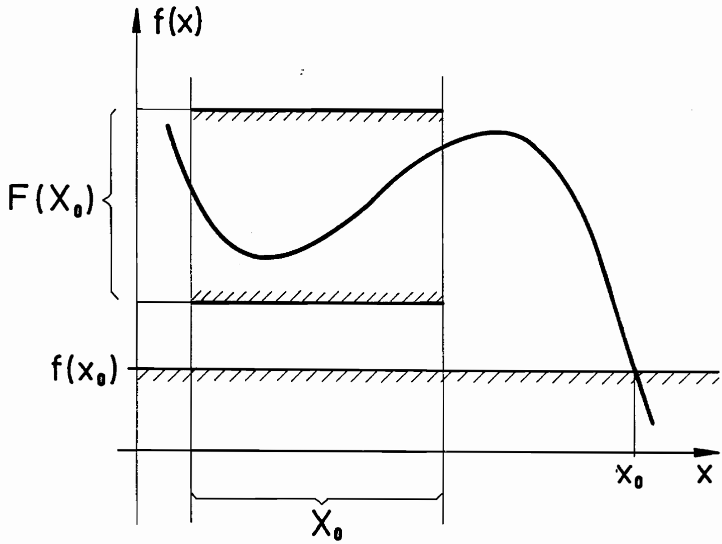


Figure 4: Exclusion of the subinterval X_0 because of $f(x_0) < F(X_0)$.

Then $\hat{x} \in X_0$ is impossible, hence X_0 can be excluded from B. This criterion of Figure 4 leads to a numerical method and an algorithm: One divides B into subintervals X_μ such that $B = \bigcup_{\mu=1}^{m} X_\mu$ and eliminates unwanted subintervals X_μ. This gives the

Result: Linear convergence to the set of all $\hat{x} \in B$ and to $f(\hat{x})$ if (*) is satisfied.

Example: In Figure 5 a) to c) this method is sketched for n = 1. The function f has two minima $\hat{x}$ in B; the subdivision is done by bisection. For the sake of simplicity the interval extension $F(X_\mu)$ is identified with $F^*(X_\mu)$ if f is monotone on X_μ. The subintervals X_μ which may (or may not) contain $\hat{x}$ are hatched; those with the mark ϑ can be omitted. A question mark ? shows uncertainty; if f is known to be strongly monotone on subintervals they can also be eliminated.

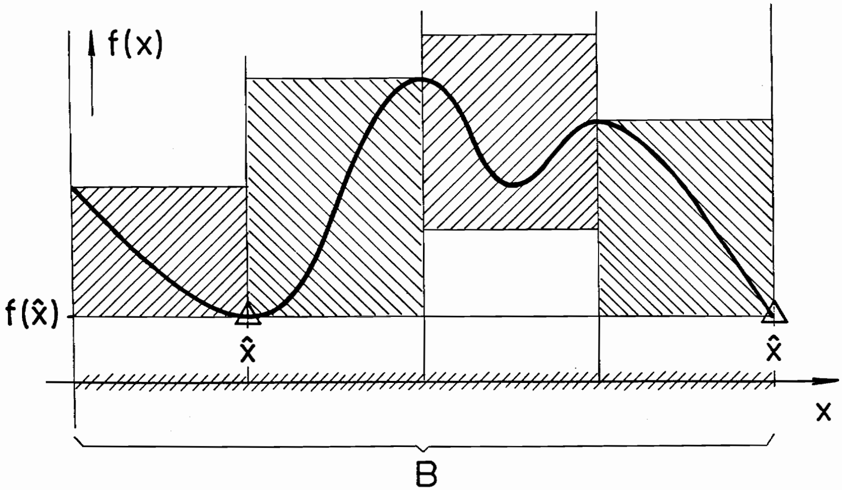
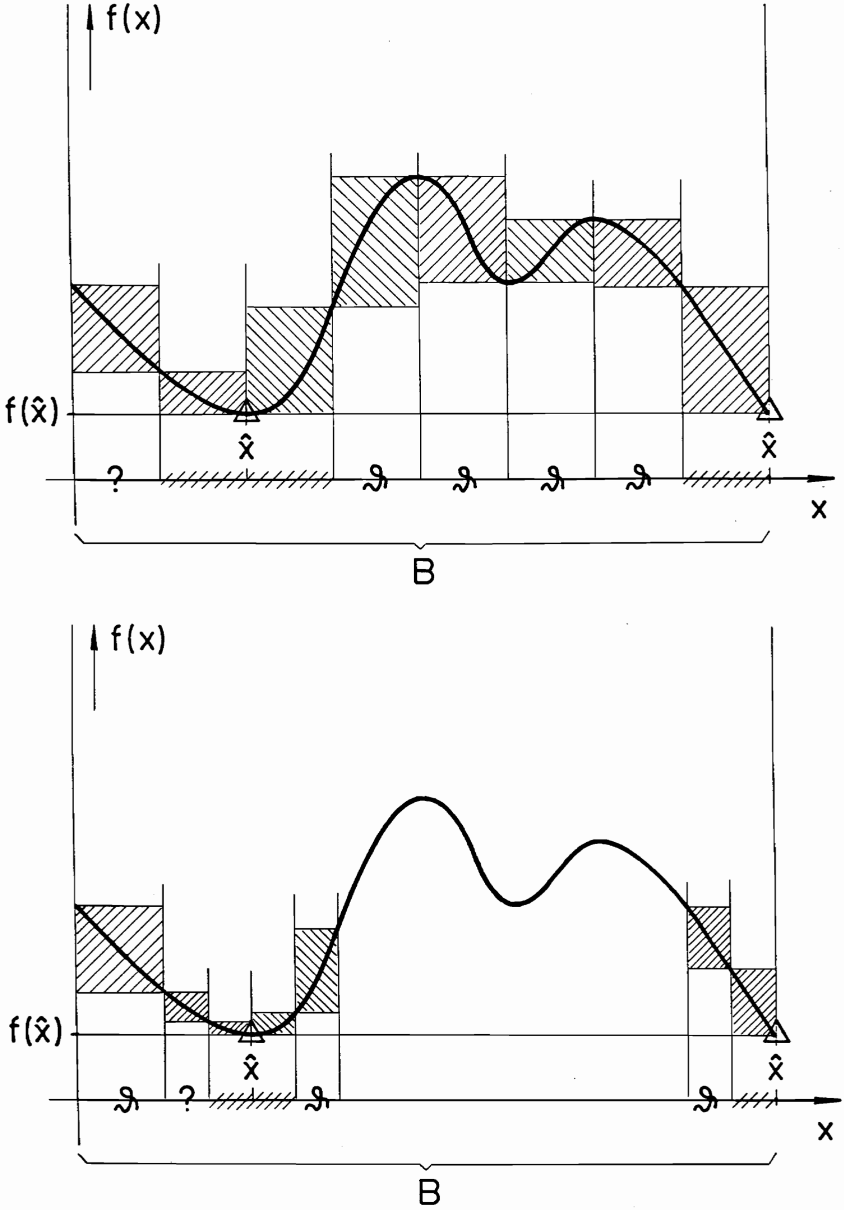


Figure 5 a): See text



Figures 5 b) and c): See text

6.3 Availability of f, F and D

Assume that to $x_0 \in B$ an interval n-vector $D = D(x_0) \in \mathbb{I}(\mathbb{R}^n)$ is known such that the following inclusion Lipschitz condition

$$(\ast)\ f(x) - f(x_0) \in D(x - x_0) \quad \text{is true for all } x \in D.$$

Conclusion: $f'(x_0) \in D$.

Important: If the computable function f is sufficiently smooth then D exists and can automatically be computed on a computer, using divided differences. Note however that D is in general not uniquely determined.

The inclusion condition (*) is sketched in Figure 6. It means

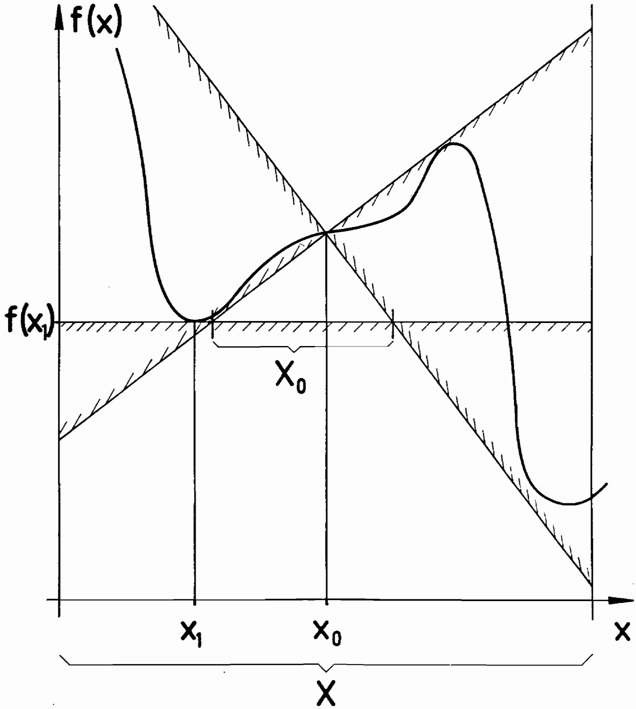


Figure 6: The inclusion condition (*)

that f is trapped in the hatched cone. This can serve as an exclusion criterion which is better than that of Figure 4.
If, in addition, a value x_1 with $f(x_1) < f(x_0)$ is known, then the subinterval X can even be split into smaller intervals which may contain $\hat{x}$ (see also Figure 6).

If, finally, (at least) one component of D does not contain zero, then $\hat{x}$ is contained in a smaller subinterval, see Figure 7.

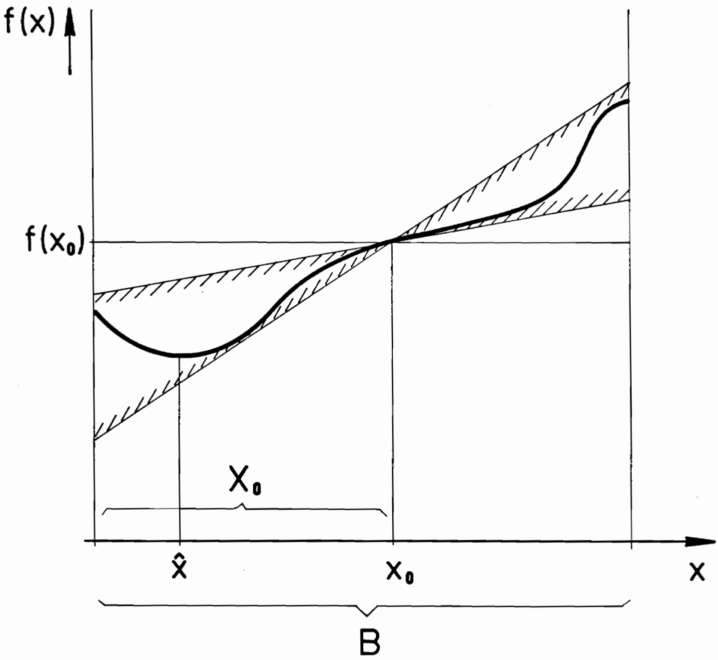


Figure 7: Inclusion criterion if D > 0 in (*)

An algorithm using the criterion based on ($\ddagger$) in addition to the previous criteria will - obviously - converge faster. It is possible to prove that ($\ddagger$) implies quadratic convergence of F(X) to F*(X) instead of the linear convergence rate of (*) (see Ratschek-Rokne, A)(1984)). This does, however, not mean that one gets quadratic convergence to $f(\hat{x})$. As above one can prove the same Result as in 6.2.

6.4 Known are f, F, f' and D

It is assumed that f and f' are computable together with interval functions F and D such that

$$f(x) \in F(X) \text{ and } f'(x) \in D(X) \quad \text{for all } x \in X \subseteq B.$$

Using the Mean Value Theorem one gets the so called "centered form"

$$f(x) \in f(z) + D(X)(x - z) \qquad \text{for all } x,z \in X \subseteq B.$$

Conclusion: $f'(x) \in D(X)$ for all $x \in X \subseteq B$.

Important: As in the case ($\ddagger$) the interval n-vector can be computed automatically.

Monotonicity check: If $\hat{x} \in \text{int}\,B$ then $f'(\hat{x}) = 0$ ($\hat{x}$ is a stationary point). Let $X_0 \subset \text{int}\,B$ and let

$$0 \notin D(X_0) \begin{cases} \text{at least in} \\ \text{one component.} \end{cases}$$

Then $\hat{x} \notin X_0$, i.e. X_0 can be discarded for the search of $\hat{x}$.

By using the centered form one can define an algorithm which converges faster than the previous ones. The same Result as in 6.2 can be obtained.

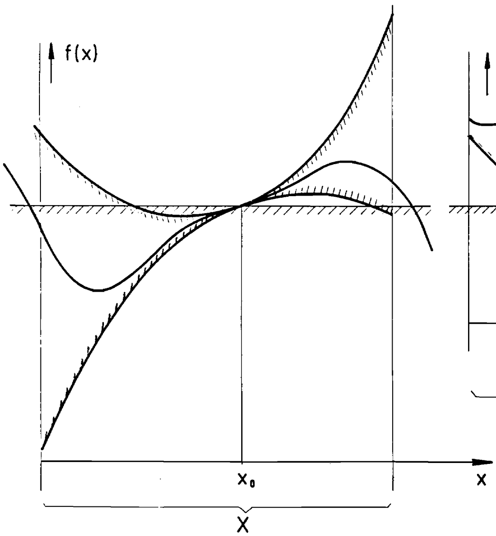
6.5 Given are $f \in F$, $f' \in D$, $f'' \in H$

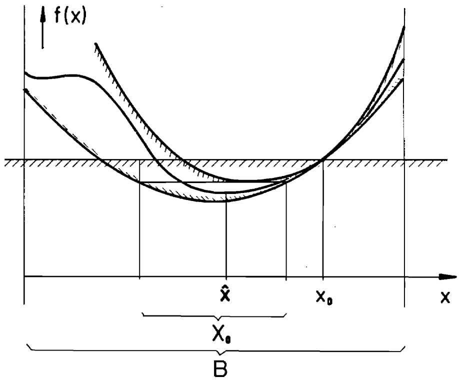
By using Taylor's Theorem one finds the following inclusion

$$(+)\quad f(x) \in f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}(x - x_0)^T H(x - x_0)$$

$$\text{for all } x_0, x \in X \subseteq B.$$

Here $H \in \mathbb{I}(\mathbb{R}^{n\times n})$. This interval extension of the Hesse matrix can automatically be computed on a computer, exactly as D.
In Figures 8 and 9 the inclusion of f(x) by (+) is sketched.





Inclusion $\hat{x} \in X_0$

Figures 8: The inclusion (+)

Figure 9: The inclusion (+) with $H > 0$ gives a better inclusion for $\hat{x}$.

Convexity check (Hansen): If $\hat{x} \in \operatorname{int} B$ then $f'(\hat{x}) = 0$ and $f''(x)$ is positiv semidefinit, hence $\operatorname{diag} f''(\hat{x}) \geqq 0$ ($\hat{x}$ is a local minimal point). Let $X_0 \subset \operatorname{int} B$ and let

$$0 > \operatorname{diag} H(X_0) \begin{cases} \text{at least in} \\ \text{one component.} \end{cases}$$

Then $\hat{x} \notin X_0$, i.e. X_0 can be omitted for the search of $\hat{x}$.

Result: There is global quadratic convergence to the set of all $\hat{x} \in B$ and to $f(\hat{x})$ if (+) is satisfied.

7. Interval Newton method

If $\hat{x} \in \operatorname{int} B$ then $\hat{x}$ is a stationary point and $f'(\hat{x}) = 0$ is true. Therefore the Newton method can (locally) be used for the evaluation of $\hat{x}$.

Assume that f' satisfies an interval Lipschitz condition

$$f'(x) - f'(y) \in H(x-y) \quad \text{for all } x,y \in B$$

with $H \in \mathbb{I}^{n\times n}(\mathbb{R})$ and assume furthermore that H^{-1} exists. Then the following simplest interval Newton method can be defined:

$$X_0 := B$$

$$\left.\begin{aligned} & x_\nu \in X_\nu \text{ arbitrary} \\ & X_{\nu+1} := X_\nu \cap (x_\nu - H^{-1} f'(x_\nu)) \end{aligned}\right\} \quad \nu = 0,1,\ldots$$

(There are more sophisticated interval Newton methods). For $n = 1$ this method is globally convergent! If f is sufficiently smooth it is always locally quadratic convergent. The interval Newton method always delivers an approximation x_ν to $\hat{x}$ together with an error bound by X_ν. Hence it is qualified for solving the interval optimization problem.

8. How to use the above mentioned properties to create interval methods and interval algorithms for optimization ?

During the last few years the development of interval methods in optimization was very fast. Nevertheless we are still far from having reached an ultimate result. Therefore only 3 (completely different) suggestions are made:

8.1 Combination of the pointwise steepest descent method with the interval Newton method

The problem in the pointwise descent methods is always how to choose the stepsize. By using the interval Newton method for n = 1 one has the big advantage that this is globally convergent. Hence the proof of global convergence of the combined method should be possible (under suitable assumptions). Only a one-dimensional Hessian interval extension is needed which makes the computational work not too expensive.

8.2 Exhaustion method

i) Use any pointwise method to get a "good" approximation $\tilde{x} \approx \hat{x}$.

ii) Find an "appropriate" neighbourhood $\tilde{X}$ to $\tilde{x}$ and use the n-dimensional interval Newton method on $\tilde{X}$ to get $\hat{X} \subseteq \tilde{X}$ with $\hat{x} \in \hat{X}$ (there exists an interval existence test for $\hat{x}$!).

iii) Exhaust the rest of B by using the above shown interval test. This exhaustion is especially well suited for parallel computing!

8.3 Dussel's method

It seems that Dussel was the first in his 1972 Ph.D.-thesis to describe a globally convergent algorithm in every detail. Unfortunately his excellent ideas have not been used since. They are (for the convex case):

i) Doing bisection. He decides which subset to omit by looking at the minimal point on the boundary between the two subsets. Hence his method is recursive in the dimension n.

ii) Instead of computing the exact minimal point in an n-1 dimensional subset he uses interval theory. Hence a (normally large) neighbourhood of this point suffices to make a decision.

iii) He avoids the trickery of creating a list by using recursive procedures(available in ALGOL or PL/1, but not in FORTRAN, yet).

9. Final remarks

Interval methods produce	FAIL SAFE ALGORITHMS .
They include automatically	ROUND OFF & DATA ERRORS.
There is an automatic	STOPPING CIRTERION .
But ...	VERY MUCH REMAINS TO BE DONE .

10. Acknowledgement

The list of references has been compiled by using the Bibliography of Dr. J. Garloff on Interval Mathematics. Dr. A. Neumaier was extremely helpful with this list and in a great number of very fruitful discussions. My very best thanks go to both of them.

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