Numerical analysis (6/7): Nonlinear (systems of) equations

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Outline

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Overview of the content

We will see methods to find solutions of nonlinear equations of the form

$$\mathbf{F}(\mathbf{x}) = \mathbf{0}$$

with $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$ and $\mathbf{x} \in \mathbb{R}^n$.
Most of the time, solutions are not known explicitly and we need numerical methods.
Finding zeros of a function has an important connection with optimization.

Objectives

- describe some of the most useful numerical methods
- study the convergence of these methods
- evaluate the efficiency i.e. the convergence speed and cost of the associated sequences
- adapt some methods to higher dimensional problems

Outline

Preliminary analysis

Problem description

- Sometimes we know how to explicitly solve some equations.
  For example
  $$x^2 - x - 1 = 0$$
  has two solutions: $\dfrac{1+\sqrt{5}}{2}$ and $\dfrac{1-\sqrt{5}}{2}$
- However, if one considers the equation
  $$\cos x = x,$$
  a mathematical theorem (which one ?) indicates that it has a unique solution between 0 and 1, but it cannot be explicitly written.
- Nevertheless, in scientific computing, an **approximation** of the solution will be sufficient with an error estimate if possible.

Preliminary analysis

Problem description

Let us consider the following 1D equation

$$f(x) = 0,\; x \in \mathbb{R}$$

where f is a real-valued function with one parameter.

- We assume that this equation admits (at least) one root r, such that $f(r) = 0$.
- The idea is to build a sequence (x_n) that converges towards r.
- Hence, the term x_n of the sequence will be an approximation of r, the accuracy depending on the choice of n.

Question

How to build the sequence (x_n) ?

Preliminary analysis

Problem description

Let us consider the following 1D equation

$$f(x) = 0, \; x \in \mathbb{R}$$

where f is a real-valued function with one parameter.

Before using a numerical method, it is better (if possible)

- to check that the equation has at least one solution
- to determine the number of roots
- to localize the roots i.e. to determine some intervals $[a_i, b_i]$ in which the considered equation has one and only one solution

Intermediate value theorem

To this end, we have

Intermediate value theorem - existence of roots

Let I be an interval in $\mathbb{R}$, f an application from I into $\mathbb{R}$, continuous on I. If there exist two elements a and b in I such that $a < b$ and $f(a)f(b) \leq 0$, then there exists $r \in [a, b]$ such that $f(r) = 0$.

Intermediate value theorem - root unicity

Let a and b two real numbers such that $a < b$ and f an application from $[a, b]$ into $\mathbb{R}$, continuous and strictly monotone on $[a, b]$. If $f(a)f(b) \leq 0$, then there exists a unique value $r \in [a, b]$ such that $f(r) = 0$.

Example

Solve on $\mathbb{R}$

$$x - 0.2\sin(x) - 0.5 = 0$$

Let f be the function defined on $\mathbb{R}$ by $f(x) = x - 0.2\sin(x) - 0.5$

The function f is continuous and differentiable on $\mathbb{R}$ and since we have for any x

$$f'(x) = 1 - 0.2\cos(x) > 0$$

this function is also strictly increasing on $\mathbb{R}$. In addition, since

$$\lim_{x\to-\infty} f(x) = -\infty \quad \text{and} \lim_{x\to+\infty} f(x) = +\infty$$

we deduce that f admits a unique root on $\mathbb{R}$.

More precisely, $f(0) = -0.5 < 0 \quad \text{and} \quad f(\pi) = \pi - 0.5 > 0$, f admits a unique root in $\mathbb{R}$ located between 0 and π.

Example

Solve in $\mathbb{R}$

$$\cos(x) = e^{-x}$$

Let f be the function defined on $\mathbb{R}$ by $f(x) = \cos(x) - e^{-x}$

The function f is continuous and differentiable on $\mathbb{R}$ and since we have for any x

$$f'(x) = -\sin(x) + e^{-x}.$$

Here it is difficult to study the sign of f' and deduce the variations of f, since we find a "similar" problem.

Example

Solve in $\mathbb{R}$

$$\cos(x) = e^{-x}$$

Let us now consider the function g defined on $\mathbb{R}$ by $g(x) = e^x \cos(x) - 1 = e^x f(x)$

The function g is continuous and differentiable in $\mathbb{R}$ and since we have for any x

$$g'(x) = e^x(\cos(x) - \sin(x)) = \sqrt{2}e^x \cos\left(x + \frac{\pi}{4}\right).$$

this function is also strictly monotone on the intervals $[\frac{\pi}{4} + k\pi, \frac{5\pi}{4} + k\pi]$, $k \in \mathbb{Z}$.

The study of the successive signs of $g(\frac{\pi}{4} + k\pi)$ allows to localize its roots.

Outline

Outline

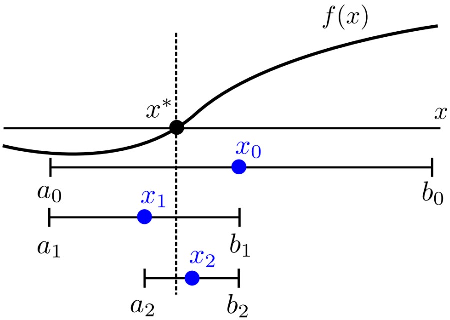
Bisection method

Principle of the bisection method

we start with an initial interval that contains a root and we build a sequence of intervals such that

- the root lies inside all the intervals
- the length of the intervals tends towards 0

One gets a converging process for localizing the roots by subdividing.



Bisection method

An interval $[a, b]$ is defined by a and b. To define the sequence of intervals, it is equivalent to fix the sequences (a_n) and (b_n) through a and b. Let $f : [a, b] \to \mathbb{R}$ be a continuous function such that $f(a) f(b) \leq 0$.

Bisection pseudo-code

$a_0 = a,\ b_0 = b$;
forall *n from* 0 *to* N **do**
  $m := \frac{(a_n + b_n)}{2}$;
  if $f(a) f(m) \leq 0$ **then**
    $a_{n+1} := a_n,\ b_{n+1} := m$;
  else
    $a_{n+1} := m,\ b_{n+1} := b_n$;
  end
end

Bisection algorithm

- The two sequences (a_n) and (b_n) satisfy by construction
  - $\forall\ n \in \mathbb{N}, \quad a_n \leq a_{n+1} \leq b_{n+1} \leq b_n$
  - $\forall\ n \in \mathbb{N}, \quad |a_n - b_n| = \frac{|a-b|}{2^n}$
  - $\forall\ n \in \mathbb{N}, \quad f(a_n)f(a) \geq 0, \quad f(b_n)f(a) \leq 0$
- consequently, the two sequences (a_n) and (b_n) are adjacent and they converge towards the same limit $r \in [a, b]$.
- since f is continuous on $[a, b]$, the sequences $(f(a_n))$ and $(f(b_n))$ converge towards $f(r)$.
- according to the sign of $f(a)$, they moreover satisfy, for any $n \in \mathbb{N}$

$$(f(a_n) \leq 0 \text{ and } f(b_n) \geq 0) \quad \text{or} \quad (f(a_n) \geq 0 \text{ and } f(b_n) \leq 0)\,.$$

- in both cases, one gets at the limit that $f(r) \leq 0$ and $f(r) \geq 0$, which implies that $f(r) = 0$.

Bisection method

Remarks

- When f is continuous on $[a, b]$ and $f(a)f(b) \leq 0$, this method converges.
- Only one evaluation per iteration of the function f is required
- Since we have

$$a_n \leq r \leq b_n, \quad \forall n \geq 0$$

  we can choose indifferently a_N or b_N as the approximation of the root, a_N being then a lower approximate value and b_N an upper approximate estimate
- we then have the following accuracy

$$|a_N - r| \leq |a_N - b_N| = \frac{|a - b|}{2^N}$$

Bisection algorithm

Remarks

- according to the expected precision ϵ , we can a priori determine the stopping index N such that

$$|a_N - b_N| = \frac{|a-b|}{2^N} < \epsilon$$

$$N \geq \text{floor}\left(\frac{\ln(|a-b|) - \ln(\epsilon)}{\ln(2)}\right) + 1$$

- This method converges even if the function f has a few roots in the initial interval.

Outline

Fixed-point methods

Principle

Searching for a solution to the equation $f(x) = 0$ can be seen as searching the solution to

$$g(x) = x$$

for example by setting

- $g(x) = x - f(x)$
- $g(x) = x - \dfrac{f(x)}{\alpha}$, with $\alpha \neq 0$
- $g(x) = x - \dfrac{f(x)}{\alpha(x)}$, with $\forall\, x \in I,\ \alpha(x) \neq 0$

Therefore, the root-finding for f amounts to searching for a fixed-point of g.

Fixed-point methods

We can then use the following algorithm

x_0 given;
forall *n from* 0 *to* ... **do**
| $x_{n+1} = g(x_n)$
end

Indeed, let us recall the following analysis result

Theorem

Let I be a closed and stable interval by g, $\xi \in I$ and (x_n) the sequence defined by the relations $x_0 = \xi$ and $x_{n+1} = g(x_n), \forall n \in \mathbb{N}$.
In addition, we assume that f is continuous on I.
If the sequence (x_n) converges, its limit is a fixed-point of g in I

A fixed-point of g is hence a root of f.

Fixed-point methods

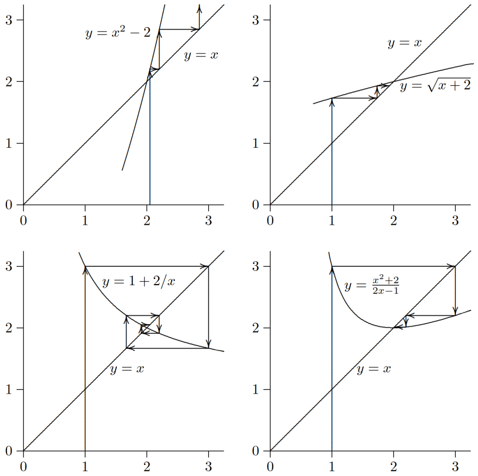


Figure: Fixed-point iterations for some nonlinear functions. From *M. T. Heath, Scientific computing: an introductory survey (2018)*

Fixed-point theorem

In particular, we have the

Fixed-point theorem

Let us assume that I is closed, g is a contraction mapping on I with ratio $k \in [0, 1)$ and I is stable by g. Then

- g admits on I a unique fixed-point $r \in I$.
- for any initial guess $\xi \in I$, the sequence (x_n), defined by $x_0 = \xi$ and the recursive relation $x_{n+1} = g(x_n)$, converges towards the fixed-point r.
- we have the following estimates

$$\forall\ n \in \mathbb{N}, \quad |x_n - r| \leq \frac{k^n}{1-k}|x_1 - x_0|$$

$$\forall\ n \in \mathbb{N}, \quad |x_n - r| \leq \frac{k}{1-k}|x_n - x_{n-1}|$$

Fixed-point methods

Example

Let f be the function defined on $I = [0, +\infty[$ by

$$f(x) = x - e^{-(1+x)}$$

This function has a unique root r between 0 and 1

Fixed-point methods

Example

Let f be the function defined on $I = [0, +\infty[$ by

$$f(x) = x - e^{-(1+x)}$$

Algorithm 1: Let g be the function defined on I by

$$g(x) = e^{-(1+x)}$$

We easily check that I is stable by g, that g is a contraction mapping on I and that I is closed

Therefore, for any $\xi \in I$, the sequence (x_n) defined by $x_0 = \xi$ and $x_{n+1} = g(x_n)$, converges towards the unique fixed-point of g which is also the root of f

Fixed-point methods

Example

Let f be the function defined on $I = [0, +\infty[$ by

$$f(x) = x - e^{-(1+x)}$$

Algorithm 2: Let us now consider h as the function defined on I by

$$h(x) = x^2 e^{(1+x)}$$

The function h admits two fixed points: 0 and r in I

Let us study, for any $\xi \in I$, the asymptotic behavior of the sequence (x_n) defined by $x_0 = \xi$ and $x_{n+1} = h(x_n)$

Fixed-point methods

Example

Let f be the function on $I = [0, +\infty[$ defined by

$$f(x) = x - e^{-(1+x)}$$

For the fixed-point function h, we show that:

- if $\xi \in [0, r[$ then the sequence (x_n) converges towards 0
- if $\xi = r$ then the sequence (x_n) is constant
- if $\xi \in]r, +\infty[$ the sequence (x_n) diverges towards $+\infty$

This second algorithm is then unadapted to get an approximation of the root r !

Fixed-point methods

Stability of the fixed-point

Let g be a map from I into I that admits a fixed-point $r \in I$.

- We say that r is an attractive or stable fixed-point if there exists $\eta > 0$ such that any sequence (x_n) defined by $x_0 \in]r - \eta, r + \eta[\cap I$, the recursive relation $x_{n+1} = g(x_n)$ converges towards r.
- We say that r is a repulsive or unstable fixed-point when for any sequence (x_n) defined by the recursive relation $x_{n+1} = g(x_n)$, there exists $n_0 \in \mathbb{N}$ such that for any $n \geq n_0$, the sequence (x_n) moves away from r.

Fixed-point methods

Theorem

Let g be a map from I into I that admits a fixed-point $r \in I$. We suppose that g is differentiable at r.

- if $|g'(r)| < 1$, then r is an attractive fixed-point.
- if $|g'(r)| > 1$, then r is a repulsive fixed-point.
- if $|g'(r)| = 1$, then both cases can arise

Remark

in the previous example, we have $|h'(r)| > 1$. The fixed point is repulsive and cannot be attained.

Outline

Convergence speed

Let (x_n) be a sequence that converges towards a number r.

- we say that the convergence speed is linear, if there exists C, $0 < C < 1$ such that

$$\lim_{n\to\infty} \frac{|x_{n+1} - r|}{|x_n - r|} = C. \tag{1}$$

- the number C is called the convergence speed.
- we say that the convergence is at least linear, if there exists C, $0 < C < 1$ such that

$$|x_{n+1} - r| \leq C\,|x_n - r| \quad \forall n \geq 0$$

Convergence speed

- we say that the convergence is of order q, if there exists $q > 1$, $C > 0$ such that

$$\lim_{n\to\infty} \frac{|x_{n+1} - r|}{|x_n - r|^q} = C$$

- we say that the convergence is at least of order q, if there exists $q > 1$, $C > 0$ such that

$$|x_{n+1} - r| \leq C\,|x_n - r|^q \quad \forall n \geq 0$$

- a second-order convergence is also called quadratic and a convergence of order 3 is said to be cubic.

Convergence speed

Practical meaning

Let us set for any $n \in \mathbb{N}$, $e_n = |x_n - r|$. The number e_n represents the error when we approximate r by x_n.

- if the convergence speed is linear then there exists $0 < C < 1$ such that $e_{n+1} \sim Ce_n$
- this means that asymptotically the error is reduced by a factor C at each iteration.
- the smaller will be the ratio C, the faster will be the convergence of the sequence

Convergence speed

Practical meaning

- if the convergence is of order $q > 1$, then there exists $C > 0$ such that $e_{n+1} \sim C e_n^q$.
- let us then set for all $n \in \mathbb{N}$, $\lambda_n = -\log_{10} e_n$.
- the number λ_n is a "measure" of the number of exact decimals of x_n.
- indeed if $e_n = 10^{-5}$ then $\lambda_n = 5$, if $e_n = 10^{-10}$ then $\lambda_n = 10$, etc...
- we have

$$\lambda_{n+1} \sim q\lambda_n.$$

  which means that asymptotically the number x_{n+1} has q times more "exact decimals" than x_n.
- the larger will be the convergence order, the faster will be the convergence of the sequence

Application to the fixed-point method

Order of convergence of a fixed-point method

Let (x_n) be a sequence defined by the recursive relation $x_{n+1} = g(x_n)$ and let r be a fixed-point of g.
If g is a three times differentiable function in I, then from the Taylor-Young formula, we have for any $n \in \mathbb{N}$

$$\begin{aligned} x_{n+1} - r &= g(x_n) - g(r) \\ &= g'(r)(x_n - r) + \frac{g''(r)}{2}(x_n - r)^2 + \frac{g'''(r)}{6}(x_n - r)^3 + o((x_n - r)^3) \end{aligned}$$

that is

$$e_{n+1} = g'(r)e_n + \frac{g''(r)}{2}e_n^2 + \frac{g'''(r)}{6}e_n^3 + o(e_n^3)$$

Application to the fixed-point method

Order of convergence of a fixed-point method

$$e_{n+1} = g'(r)e_n + \frac{g''(r)}{2}e_n^2 + \frac{g'''(r)}{6}e_n^3 + o(e_n^3)$$

Several cases then appear

- if $g'(r) \neq 0$ and $|g'(r)| < 1$, then $e_{n+1} \sim Ce_n$ with $C = |g'(r)|$.
  The sequence (x_n) converges linearly to r.
- if $g'(r) = 0$ and $g''(r) \neq 0$, then $e_{n+1} \sim Ce_n^2$ with $C = \frac{|g''(r)|}{2}$.
  The sequence (x_n) is convergent of order 2.
- if $g'(r) = g''(r) = 0$ and $g'''(r) \neq 0$, then $e_{n+1} \sim Ce_n^3$ with $C = \frac{|g'''(r)|}{6}$.
  The sequence (x_n) is converging of order 3.
- and so on, if we assume more smoothness on g.

Outline

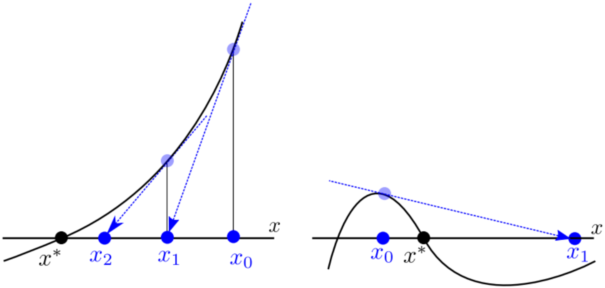
The Newton method

Description of the method

- if f is an affine function

$$f(x) = ax + b \quad (a \neq 0)$$

  the root is $r = -b/a$.
- the idea is to substitute f by an affine approximation $\rightarrow$ we can use its tangent.



The Newton method

Description of the method

Let us assume that f is a function defined on an interval I, differentiable on I and such that it has a root r in I

- let x_0 be a point I close enough to the root r
- we then have

$$\begin{aligned} f(x) &= f(x_0) + f'(x_0)(x - x_0) + o(x - x_0) \\ &= f_{x_0}(x) + o(x - x_0) \end{aligned}$$

with $f_{x_0}(x) = f'(x_0)(x - x_0) + f(x_0)$

The Newton method

Description of the method

- the affine function f_{x_0} admits a root x_1 if and only if $f'(x_0) \neq 0$, and in this case

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

- we can expect then that x_1 will be closer to the root r than x_0 i.e. that x_1 is a better estimate of r
- we can then iterate with x_1 instead of x_0 and so on...
- we expect to improve the approximation of the root r through successive iterations.

The Newton method

Newton's algorithm

x_0 given;
forall n *from* 0 *to* ... **do**

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

end

Remarks

- to have a well-defined sequence (x_n), we must have $f'(x_n) \neq 0$, $\forall n \in \mathbb{N}$.
- at each iteration, we have to evaluate two functions: computation of $f(x_n)$ and computation of $f'(x_n)$
- the Newton method is a fixed-point method with $g(x) = x - \frac{f(x)}{f'(x)}$

Convergence of the Newton method

Theorem

Let f be an application from I into I and $r \in I$ a root of the function f. We assume that f is twice differentiable in a neighborhood of r and that $f'(r) \neq 0$.
Then, there exists $\eta > 0$ such that for any $x_0 \in]r - \eta, r + \eta[\cap I$ the Newton method generates a well-defined sequence (x_n) which converges at least quadratically towards r.

Indeed

$$g'(x) = 1 - \frac{(f'(x))^2 - f(x)f'(x)}{(f'(x))^2}$$

and so $g'(r) = 0$

Convergence of the Newton method

Remarks

- this result indicates that if x_0 is close enough to r (and if $f'(r) \neq 0$) then the method converges
- when there is convergence, it is fast (at least of order 2)
- if x_0 is not close enough to r, then divergence may occur
- in practice, there is generally no way to know if x_0 is close enough to r
- if the derivative does not exist or is discontinuous at the root, Newton's method may fail

Newton method

Example

Example : $x^2 = a$ Let $a > 0$

- we search for an approximation of $\sqrt{a}$
- here $f(x) = x^2 - a$ and the Newton algorithm writes

$$x_{n+1} = x_n - \frac{x_n^2 - a}{2x_n} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$$

- it can be easily shown that for any $x_0 > 0$ this sequence converges towards $\sqrt{a}$

Newton method

Example

Example : $x^2 = a$ for $a = 2$ and $x_0 = 1$ ones gets

$$\begin{aligned} x_0 &= 1 \\ x_1 &= \frac{3}{2} = 1.5 \\ x_2 &= \frac{17}{12} = 1.41666666666666\ldots \\ x_3 &= \frac{577}{408} = 1.41421568627450\ldots \\ x_4 &= \frac{665857}{470832} = 1.41421356237468\ldots \end{aligned}$$

Newton method

Example : $x^2 = a$

for $a = 2$ and $x_0 = 1$ one gets

$$\begin{aligned} x_0 &= 1 \\ x_1 &= \frac{3}{2} = 1.5 \\ x_2 &= \frac{17}{12} = 1.41666666666666\ldots \\ x_3 &= \frac{577}{408} = 1.41421568627450\ldots \\ x_4 &= \frac{665857}{470832} = 1.41421356237468\ldots \end{aligned}$$

let us remind us that

$$\sqrt{2} = 1.414213562373095\ldots$$

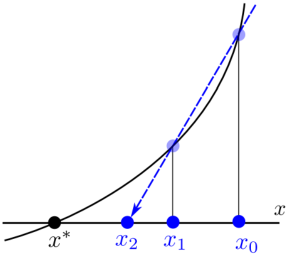
Outline

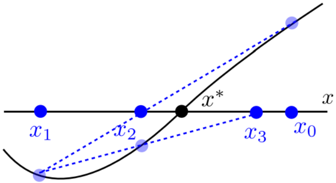
Another remark on Newton method

One Newton iteration $x_{n+1} = x_n - f(x_n)/f'(x_n)$ requires the evaluation of two functions: $f(x_n)$ and $f'(x_n)$.

- the derivative f must be known and we must be able to implement its evaluation f'
- we could also use

$$f'(x) \simeq \frac{f(x+h) - f(x)}{h}$$





The secant method

A new method

Hence, one gets a close form method for evaluating f' :

x_0 given;
forall n *from* 0 *to* ... **do**

$$x_{n+1} = x_n - \frac{f(x_n)h_n}{f(x_n+h_n)-f(x_n)}$$

end

Remarks

- this method is well-defined if at each iteration $f(x_n + h_n) - f(x_n) \neq 0$
- the numerical step h_n can be different at each iteration
- at each step, we always have two evaluations: computation of $f(x_n)$ and $f(x_n + h_n)$

The secant method

to avoid this double evaluation, one can set

$$h_n = x_{n-1} - x_n \quad \forall n \geq 0$$

Indeed, if (x_n) converges, then (h_n) converges towards 0 and at each iteration we only have one evaluation: computation of $f(x_n)$ (if the algorithm is correctly written!)

forall *n from* 0 *to* ... **do**

$$x_{n+1} = x_n - \frac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}$$

end

the resulting algorithm is called the secant method

The secant method

Analysis of the method

Let us assume that f is a function defined on an interval I and that it has a root r in I

- let x_0 and x_1 be two points in I close enough to the root r
- we substitute in a neighborhood of x_1 the function f by the line passing through the points $(x_1, f(x_1))$ and $(x_0, f(x_0))$ of equation

$$f_{x_1}(x) = \left(\frac{f(x_1) - f(x_0)}{x_1 - x_0} \right) (x - x_1) + f(x_1)$$

The secant method

Analysis of the method

- the affine function f_{x_1} admits a root x_2 if and only if $f(x_1) - f(x_0) \neq 0$, and in this case

$$x_2 = x_1 - f(x_1)\left(\frac{x_1 - x_0}{f(x_1) - f(x_0)}\right)$$

- we can expect that x_2 is closer to the root r than both x_0 and x_1
- we can then iterate with x_2 and x_1 and so on...
- we expect to improve the approximation of the root r by successive approximations.

The secant method

The secant method algorithm

x_0 x_1 given;
forall *n from* 0 *to* ... **do**

$$x_{n+1} = x_n - f(x_n)\frac{(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}$$

end

Remarks

- to get a well-defined sequence (x_n), we must have that $f(x_n) \neq f(x_{n-1})$ for all $n \in \mathbb{N}$.
- at each iteration, we have one evaluation: computation of $f(x_n)$
- the convergence analysis is similar to Newton's method,

Convergence of the secant method

Theorem

Let f be a map from I in I and $r \in I$ a root of the function f. We assume that f is twice continuously differentiable in a neighborhood of r and that $f'(r) \neq 0$.
Then, if (x_0, x_1) are sufficiently close to r the secant method generates a sequence (x_n) which is well-defined and converging towards r.
The error satisfies

$$|e_{n+1}| \leq C|e_n||e_{n-1}|$$

In this case, the convergence is at least of order $\frac{1+\sqrt{5}}{2} = 1.618...$

Outline

Comparison between the algorithms

Bisection

- the method is converging
- only one evaluation at each iteration
- convergence speed is linear and therefore slow

Newton

- fast convergence when it converges
- not to sensitive to round-off errors if $f'(r)$ is not too small
- can diverge if the initial guess is not correctly chosen
- requires the evaluation of the derivative
- two evaluations at each iteration

Secant

- relatively fast convergence when the convergence occurs
- requires one evaluation of the function at each iteration
- can diverge if the initial guess is not correctly calibrated

Example

Resolution of $x - 0.2 \sin x - 0.5 = 0$ with the four algorithms

	Bisection $x_{-1} = 0.5$ $x_0 = 1.0$	Secant $x_{-1} = 0.5$ $x_0 = 1.0$	Newton $x_0 = 1$	Fixed-point $x_0 = 1$ $x = 0.2 \sin x + 0.5$
1	$0,75$	$0,5$	$0,5$	$0,50$
2	$0,625$	$0,61212248$	$0,61629718$	$0,595885$
3	$0,5625$	$0,61549349$	$0,61546820$	$0,612248$
4	$0,59375$	$0,61546816$	$0,61546816$	$0,614941$
5	$0,609375$			$0,61538219$
6	$0,6171875$			$0,61545412$
7	$0,6132812$			$0,61546587$
8	$0,6152343$			$0,61546779$
9	$0,6162109$			$0,61546810$
10	$0,6157226$			$0,61546815$
11	$0,6154785$			
12	$0,6153564$			
13	$0,6154174$			
14	$0,6154479$			
15	$0,6154532$			
16	$0,61547088$			
17	$0,61546707$			
18	$0,61546897$			
19	$0,615468025$			
20	$0,615468502$			

Outline

Convergence acceleration

Principle

Being given a sequence (x_n) that converges to r, accelerating the convergence consists in replacing the initial sequence by a sequence (y_n) that converges faster than (x_n) towards r, i.e; satisfying

$$\lim_{n \to +\infty} \frac{y_n - r}{x_n - r} = 0.$$

Example

if (x_n) converges linearly then (y_n) will converge faster or to a higher order.

Relaxation method

Let us consider a fixed-point method

$$x_{n+1} = g(x_n)$$

that slowly converges or diverges

The equation that we are looking for $x = g(x)$ can also be written for any $\alpha \neq -1$

$$x + \alpha x = g(x) + \alpha x$$

or

$$x = \frac{g(x) + \alpha x}{1 + \alpha} = G(x)$$

We can then think of using a fixed-point

$$y_{n+1} = G(y_n)$$

Relaxation method

From the previous results, this method will converge as soon as y_0 is close to the fixed-point r and when

$$|G'(r)| = \left| \frac{g'(r) + \alpha}{\alpha + 1} \right| < 1$$

The convergence will be better when $|G'(r)|$ is small

Since we are free to choose the relaxation parameter α, the idea is to take it as close as possible to $-g'(r)$!

Aitken acceleration method

Hypothesis

Let (x_n) be a sequence converging to r and such that

$$x_{n+1} - r = k\,(x_n - r) \text{ where } 0 < k < 1$$

We have

$$\begin{aligned} x_{n+1} - r &= k\,(x_n - r)\,, \\ x_{n+2} - r &= k\,(x_{n+1} - r)\,. \end{aligned}$$

and by difference one gets

$$x_{n+2} - x_{n+1} = k\,(x_{n+1} - x_n)\,.$$

Aitken acceleration method

The principle

Let (x_n) be a sequence converging to r and such that

$$x_{n+1} - r = k\,(x_n - r) \text{ where } 0 < k < 1$$

By reporting then in the first equation written as

$$r = x_n + \frac{x_{n+1} - x_n}{1 - k}$$

we have

$$r = x_n - \frac{(x_{n+1} - x_n)^2}{x_{n+2} + x_n - 2x_{n+1}}.$$

three consecutive terms of the sequence are then enough to get r !

Aitken acceleration method

The principle

But the hypothesis is very strong and unrealistic.

The idea of Aitken is to generalize this remark to sequences that converge linearly that is

$$x_{n+1} - r = k_n \,(x_n - r) \quad \text{with} \lim_{n\to\infty} k_n = k \in [0, 1[\,.$$

For n large, k_n is almost constant, and so the number

$$y_n = x_n - \frac{(x_{n+1} - x_n)^2}{x_{n+2} + x_n - 2x_{n+1}}$$

should be close to r.

Aitken acceleration method

Theorem

Let (x_n) be a sequence that converges linearly to r.Then the sequence (y_n) defined by

$$y_n := x_n - \frac{(x_{n+1} - x_n)^2}{x_{n+2} + x_n - 2x_{n+1}}$$

satisfies

$$\lim_{n\to\infty} \frac{y_n - r}{x_n - r} = 0.$$

The Aitken process allows to accelerate the convergence of a sequence which is linearly converging.

Aitken acceleration method

Remark:

For the computations, we will use the equivalent expression

$$y_n = x_{n+1} + \frac{1}{\frac{1}{x_{n+2}-x_{n+1}} - \frac{1}{x_{n+1}-x_n}}$$

this one having a better behavior regarding the round-off errors due to the use of a computer.

Steffensen algorithm

The principle

Let (x_n) be defined by:

$$x_{n+1} = g(x_n) \ \forall n \geq 0$$

and let us assume that (x_n) converges at least linearly to r.

This convergence can be improved bu using the Aitken method.

The idea is to use y_n (which is *a priori* closer to the limit r than x_n) instead of x_n in the Aitken algorithm to expect a double acceleration...

Steffensen algorithm

One gets the algorithm

x_0 given;
forall *n from* 0 *to* ... **do**

$$y_n := g(x_n);$$
$$z_n := g(y_n);$$
$$x_{n+1} := x_n - \frac{(y_n - x_n)^2}{z_n - 2y_n + x_n}$$

end

Steffensen algorithm

Remarks

- this algorithm is a new fixed-point algorithm

$$x_{n+1} = G\left(x_n\right) \text{ with } G\left(x\right) = x - \frac{\left(g\left(x\right) - x\right)^2}{g\left(g\left(x\right)\right) - 2g\left(x\right) + x}.$$

- we show that if $g'\left(r\right) \neq 0$, then $G'(r) = 0$. The algorithm associated with G converges then quadratically.
- hence, compared with the algorithm associated to g
  - we accelerate the convergence when it is converging
  - we have a converging process, even if $\left|g'\left(r\right)\right| \geq 1$.
- it must be noticed that if the algorithm for G converges faster that the one for g, each iteration needs two function evaluations: we have to pay the price !

Outline

Problem description

Multivariate function

Let us consider the equation

$$F(X) = 0$$

where $F : \mathbb{R}^N \mapsto \mathbb{R}^N$ or in terms of scalar equations

$$\begin{cases} f_1(x_1, x_2, \dots, x_N) & = 0 \\ f_2(x_1, x_2, \dots, x_N) & = 0 \\ \vdots & \vdots \\ f_N(x_1, x_2, \dots, x_N) & = 0 \end{cases}$$

The Newton-Raphson method

- the Newton-Raphson method is a generalization to higher-dimensional problems of the one-dimensional Newton method

$$x_{n+1} = x_n - (f'(x_n))^{-1} f(x_n)$$

- it involves the Jacobian matrix of F:

$$F'(X_n) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \frac{\partial f_N}{\partial x_2} & \cdots & \frac{\partial f_N}{\partial x_N} \end{pmatrix}$$

  all the derivatives being evaluated at point X_n.
  The Newton-Raphson method formally writes down

$$X_{n+1} = X_n - [F'(X_n)]^{-1} F(X_n)$$

Taylor Series for vector functions

Theorem

Let $X = (x_1, x_2, \ldots, x_n)^T$, $F = (f_1, f_2, \ldots, f_m)^T$, and assume that $F(X)$ has bounded derivatives up to order at least two. Then for a direction vector $P = (p_1, p_2, \ldots, p_n)^T$, the Taylor expansion for each function f_i in each coordinate x_j yields

$$F(X+P) = F(X) + F'(X)P + \mathcal{O}\left(\|P\|^2\right),$$

where $F'(X)$ is the Jacobian matrix of first derivatives of F at X. Thus we have

$$f_i(X+P) = f_i(X) + \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_j} p_j + \mathcal{O}\left(\|P\|^2\right), \quad i = 1, \ldots, m$$

For a small $P = R - X_n$, we have $0 = F(X_n + P) \approx F(X_n) + F'(X_n)(R - X_n)$.
We then define δ_n such as $F(X_n) + F'(X_n)\delta_n = 0$

The Newton-Raphson method

In a practical computation, we do not explicitly compute the inverse of the Jacobian matrix which would be too expensive. We prefer to write the algorithm under the following form

X_0 given;
forall *n from* 0 *to* ... **do**
    Solve the linear system $F'(X_n)\delta_n = -F(X_n)$;
    $X_{n+1} = X_n + \delta_n$;
end

The Newton-Raphson method

Remarks :

- the choice of the initial guess is crucial and the risk that the algorithm diverges truly exists.
- the convergence is second-order and therefore is really fast (when it converges!)
- the Newton-Raphson method is expensive since at each iteration one must
  - evaluate $N^2 + N$ functions (the N^2 partial derivatives of the Jacobian matrix, plus the N coordinates functions)
  - solve $N \times N$ the linear system (with a dense matrix!)

The Broyden method

Principle

- in the Newton-Raphson method, the computation of the Jacobian matrix is highly expensive
- we will then only determine an approximate value B_n at each iteration
- we have seen that the secant method could be deduced from the Newton method by approximating

$$f'(x_n) \quad \text{by} \quad \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

- in higher dimension N, we will just force the sequence of matrices (B_n) to verify the same relation

$$B_n(X_n - X_{n-1}) = F(X_n) - F(X_{n-1})$$

The Broyden method

Remarks:

- this relation does not allow us to uniquely define the matrix B_n (n equations for n^2 unknowns)
- it only imposes its value in one direction
- Broyden proposed to update B_n to B_{n+1} by simply adding a rank-one matrix

$$B_{n+1} = B_n + \frac{(\delta F_n - B_n \delta X_n)(\delta X_n)^T}{\|\delta X_n\|^2}$$

  where we introduced $\delta X_n = X_{n+1} - X_n$ and $\delta F_n = F(X_{n+1}) - F(X_n)$.
- we immediately verify that the sequence of defined matrices (B_n) then satisfy the relation.

The Broyden method

The Broyden algorithm

X_0 and B_0 given;
forall *n from* 0 *to* . . . **do**

  Solve the linear system $B_n \delta_n = -F(X_n)$;
  $X_{n+1} = X_n + \delta_n$;
  $\delta F_n = F(X_{n+1}) - F(X_n)$;
  $$B_{n+1} = B_n + \frac{(\delta F_n - B_n \delta_n)(\delta_n)^T}{\|\delta_n\|^2};$$

end

The Broyden method

Remarks:

- we can take the initial matrix as $B_0 = Id$; after a certain time, the matrix becomes a suitable approximation of the Jacobian matrix.
- it can be proved that in general and as for the secant method, the convergence is superlinear.
- The sequence of matrices (B_n) does not necessarily converge towards the Jacobian of F.

Summary

We have seen a few methods to find roots of 1D non-linear equations.

- the fixed-point theory is a fundamental concept to develop algorithms,
- they are methods to accelerate convergence (Aitken-acceleration)
- built-in methods combine the bisection, Newton and secant methods

In two or more dimensions the situtation is more complicated

- Newton method can still be used, but is very costly
- Cheaper methods can be devised by approximating the Jacobian
- Root-finding is strongly linked to optimization: zeros of the Jacobian help to detect extrema of functions