# Numerical Methods 2. Solution of nonlinear equations

## Solution by interval halving (bisection method)

Let $f:[a,b]\to\mathbf{R}$ be continuous, assume that $f(a)<0,\quad f(b)>0$. Let us look for a solution of the equation

$$f(x)=0$$

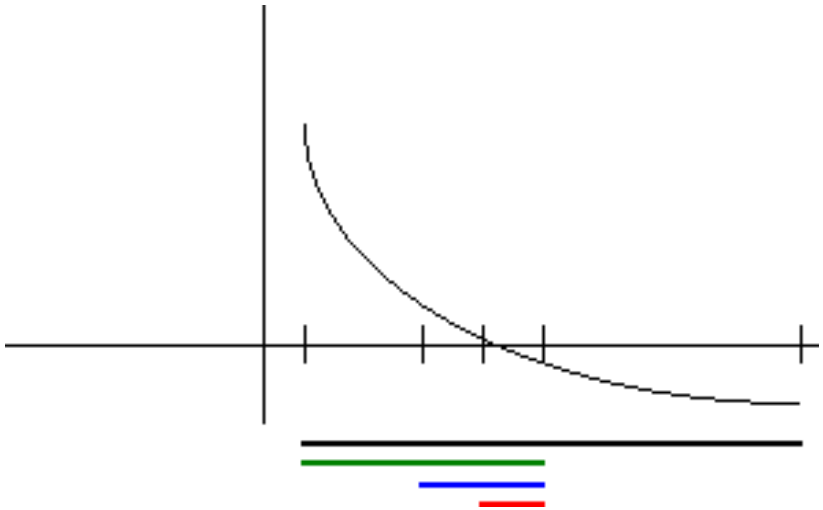
in the interval $[a,b]$.

Bolzano's theorem: If $f$ is continuous on the finite, closed interval $[a,b]$, and the signs of $f(a)$ and $f(b)$ are different, e.g. $f(a)<0,\quad f(b)>0$, then $f$ has (at least one) zero in this interval.

Let us systematically halve the interval $[a,b]$ by taking the subinterval which has the property that the values of $f$ at the endpoints of the subinterval have different signs. Denote by $x_n$ the centre of the subinterval obtained in the $n$th step. Then this sequence converges to a zero (one of the zeroes) of the above equation. The speed of convergence is of a geometric sequence with quotient ½.

**Solution by interval halving (bisection method)**

The algorithm is illustrated by the following figure:



*Error estimation*: Defining $x_0 := \dfrac{a+b}{2}$, it is obvious that:

$$\left| x_n - x^* \right| \leq \frac{b-a}{2^n}$$

**The method based on Banach's fixed point theorem**

Let $X$ be a Banach space, let $f : X \to X$ be a mapping, and look for a vector $x$ such that

$$x = f(x)$$

(a **fixed point** of the mapping $f$).

**Banach's fixed point thorem**: Let $X$ be a Banach space, let $f : X \to X$ be a **contraction** in $X$, i.e. assume that there exists a number $0 \le q < 1$ such that $\| f(x) - f(y) \| \le q \cdot \| x - y \|$ is valid for every $x, y \in X$. Then $f$ has an unique fixed point $x \in X$, and this is the limit of the following, recursively defined *iteration sequence*:

$$x_0 \in X, \quad x_{n+1} := f(x_n) \qquad (n = 0,1,2, \dots)$$

In particular, if $f : \mathbf{R} \to \mathbf{R}$ a function for which $\max | f'(x) | < 1$ is satisfied, then $f$ is a contraction, since Lagrange's mean value theorem implies that

$$| f(x) - f(y) | = | f'(\xi) | \cdot | x - y | \le (\max | f' |) \cdot | x - y |.$$

**Proof of the fixed point theorem**: The distance of two consecutive terms:

$$\| x_{n+1} - x_n \| = \| f(x_n) - f(x_{n-1}) \| \le q \| x_n - x_{n-1} \| = q \| f(x_{n-1}) - f(x_{n-2}) \| \le q^2 \| x_{n-1} - x_{n-2} \| \le$$

$$\ldots \le q^n \| x_1 - x_0 \|$$

Utilizing this estimation, we show that $(x_n)$ is a Cauchy sequence in $X$:

$$\| x_{n+k} - x_n \| = \| x_{n+k} - x_{n+k-1} + x_{n+k-1} - x_{n+k-2} + \ldots + x_{n+1} - x_n \| \le$$

$$\le \| x_{n+k} - x_{n+k-1} \| + \| x_{n+k-1} - x_{n+k-2} \| + \ldots + \| x_{n+1} - x_n \| \le$$

$$\le (q^{n+k-1} + q^{n+k-2} + \ldots + q^n) \cdot \| x_1 - x_0 \| \le$$

$$\le (q^n + q^{n+1} + q^{n+2} + \ldots) \cdot \| x_1 - x_0 \| = \frac{q^n}{1-q} \cdot \| x_1 - x_0 \| \to 0$$

(when $n \to +\infty$.) Therefore the sequence is convergent, $x_n \to x \in X$. We show that $x$ is a fixed point of $f$. By definition: $x_{n+1} = f(x_n)$ The left hand side obviously tends to $x$. The right-hand side tends to $f(x)$, since $f$ is continuous. This implies that $x = f(x)$.

Finally, prove the uniqueness of the fixed point. If $x, y$ were two *different* fixed points, then

$$0 < \| x - y \| = \| f(x) - f(y) \| \le q \cdot \| x - y \| < \| x - y \|$$

would be valid, which is impossible.

**Iteration based on Banach's fixed point theorem, examples:**

1. Solve the equation $\boxed{x = \frac{1}{2}\cos x.}$

The function defined by $f(x) := \frac{1}{2}\cos x$ is a contraction in **R**, since $|f'(x)| = \frac{1}{2}|\sin x| \le \frac{1}{2}$. Thus, an unique fixed point exists, and e.g. the following sequence converges to this: $x_0 := 0$, $x_{n+1} := \frac{1}{2}\cos x_n$. The first terms of the sequence are as follows (with four decimal digits): 0.0000, 0.5000, 0.4387, 0.4526, 0.4496, 0.4502, 0.4501, 0.4501, 0.4501, ...

2. Let $B \in \mathbf{M}_{N\times N}$, $g \in \mathbf{R}^N$ be given, and solve the linear system of equations $\boxed{x = Bx + g.}$

If $\| B \| < 1$ (with respect to an arbitrary matrix norm induced by a vector norm), then the mapping $f(x) := Bx + g$ is a contraction, since

$$\| f(x) - f(y) \| = \| Bx + g - By - g \| \le \| B \| \cdot \| x - y \|$$

In this case, there exists a unique fixed point, and the vector sequence defined by $x_0 := \mathbf{0}$, $x_{n+1} := Bx_n + g$ converges to the fixed point.

**Newton's method for univariate functions**

Let $f:(a,b)\to\mathbf{R}$ be a given function. Solve the equation

$$\boxed{f(x)=0}$$

in the interval $(a,b)$.

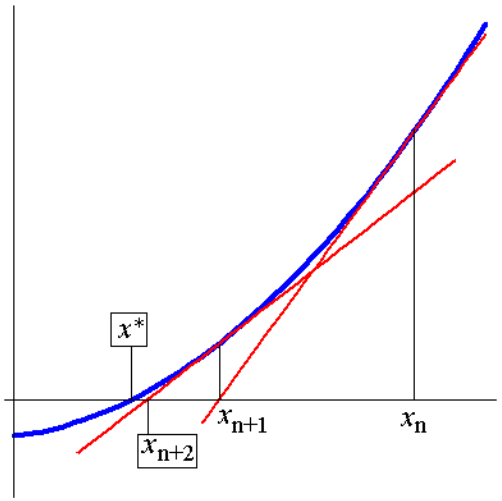
**Newton's method**: If $x_n$ is an approximate solution, then define an improved approximation to be the zero of the tangent line at $x_n$. The equation of the tangent line is:

$y=f(x_n)+f'(x_n)\cdot(x-x_n)$, whence:

$$\boxed{x_{n+1}=x_n-\frac{f(x_n)}{f'(x_n)}\quad (n=0,1,2,\ldots)\qquad\qquad (x_0\in(a,b)\text{: initial approximation})}$$

## Newton's method for univariate functions

Illustration of then method ($x^*$ denotes the exact solution):




If $f$ is twice continuously differentiable, $f$ has a zero in $(a,b)$, and $f'(x^*) \neq 0$ is valid, then Newton's iteration **quadratically converges** to $x^*$ for arbitrary initial approximation $x_0$ which is sufficiently close to the exact solution $x^*$, i.e. for a proper positive constant $C > 0$:

$$\boxed{|x_{n+1} - x^*| \leq C \cdot |x_n - x^*|^2}$$

**Proof**: We utilize *Lagrange's mean value theorem* twice:

$$x_{n+1} - x^* = x_n - x^* - \frac{f(x_n) - f(x^*)}{f'(x_n)} = x_n - x^* - \frac{f'(t)(x_n - x^*)}{f'(x_n)} =$$

$$= \frac{f'(x_n) - f'(t)}{f'(x_n)} \cdot (x_n - x^*) = \frac{f''(s)}{f'(x_n)} \cdot (x_n - t) \cdot (x_n - x^*)$$

Since $f'(x^*) \neq 0$, the derivative function differs from zero in a closed neighbourhood of $x^*$. In this neighbourhood:

$$|x_{n+1} - x^*| \leq \frac{\max|f''|}{\min|f'|} \cdot |x_n - t| \cdot |x_n - x^*| \leq \frac{\max|f''|}{\min|f'|} \cdot |x_n - x^*|^2 = C \cdot |x_n - x^*|^2$$

**Newton's method, example**:

Let $A$ be a fixed positive number, and define: $f(x) := x^2 - A$. $(\Rightarrow \quad f'(x) = 2x)$
Now the unique positive solution of the equation

$$f(x) = 0$$

is $x = \sqrt{A}$.

Starting form an arbitrary initial approximation $x_0 > 0$ (e.g. $x_0 := A$), we arrive at the following recursion:

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

The sequence converges to $\sqrt{A}$ *extremely rapidly*, requiring only additions and divisions.

*Remark*: Newton's method can be applied to the computation of any root in a similar way.

**Some variants of Newton' method**

The main difficulty: the computation of the derivatives.

**The secant method**: Here $f'(x_n) \approx \dfrac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$, which results in the recursion:

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

If $f$ is twice continuously differentiable, $f$ has a root $x^*$ in $(a,b)$, and $f'(x^*) \neq 0$, then the secant method defines an iteration which converges to $x^*$ provided that the initial approximations $x_0$, $x_1$ are sufficiently close to the exact solution.
The speed of convergence is **at least** that of a geometrical sequence, i.e.

$$|x_n - x^*| \leq C \cdot q^n$$

for some $C > 0,\ 0 < q < 1$

*Remark*: In fact, the speed of convergence is faster (*superlinear convergence*).

**Some variants of Newton' method**

**Steffensen's method**:

Assume that the function $f:\mathbf{R}\to\mathbf{R}$ is twice continuously differentiable and has a unique root $x^*$. Assume also that $f'(x^*)\neq 0$. Then for any initial approximation $x_0$ which is sufficiently close to $x^*$, the following recursive sequence is quadratically converges to $x^*$:

$$x_{n+1} := x_n - \frac{f(x_n)^2}{f(x_n + f(x_n)) - f(x_n)} \qquad (n = 0,1,2,\ldots)$$

*Remark*: Both the secant method and Steffensen's method require computing the values of the function $f$ but not of the derivatives.

**Proof of the convergence of Steffensen's method**: Utilizing Lagrange's mean value theorem:

$$f(x_n + f(x_n)) - f(x_n) = f'(t)\cdot(x_n + f(x_n) - x_n) = f'(t)\cdot f(x_n)$$

therefore

$$x_{n+1} - x^* = x_n - x^* - \frac{f(x_n)}{f'(t)} = x_n - x^* - \frac{f(x_n) - f(x^*)}{f'(t)} = x_n - x^* - \frac{f'(s)}{f'(t)}(x_n - x^*) =$$
$$= \frac{f'(t) - f'(s)}{f'(t)}\cdot(x_n - x^*) = \frac{f''(w)}{f'(t)}\cdot(t-s)\cdot(x_n - x^*)$$

Since $f'(x^*) \neq 0$, therefore the derivative function differs from a closed neighbourhood of $x^*$, and here:

$$|x_{n+1} - x^*| \leq \frac{\max|f''|}{\min|f'|}\cdot|t-s|\cdot|x_n - x^*| \leq \frac{\max|f''|}{\min|f'|}\cdot|x_n - x^*|^2 = C\cdot|x_n - x^*|^2$$

## Differentiation of functions mapping between Banach spaces

Let $X,Y$ be Banach spaces. The mapping $F : X \to Y$ is said to be **differentiable** at the point $x \in X$ and its **derivative** is the **bounded linear operator** $A : X \to Y$, if for any vector $h$ chosen from a proper neighbourhood of $\mathbf{0}$, the following equality is valid:

$$F(x+h) = F(x) + Ah + o(h)$$

where $o(h)$ is an expression such that $\frac{o(h)}{||h||} \to \mathbf{0} \quad (h \to \mathbf{0})$.

Notations: $F'(x)$ or $DF(x)$.

*Example*: $F : \mathbf{R}^N \to \mathbf{R}$, $F(x) := \langle Ax, x \rangle$ (where $A \in \mathbf{M}_{N \times N}$ is a self-adjoint matrix), then:

$$F(x+h) = \langle A(x+h), x+h \rangle = \langle Ax, x \rangle + 2\langle Ax, h \rangle + \langle Ah, h \rangle = F(x) + \langle 2Ax, h \rangle + O(h^2).$$

Thus, $F'(x) = 2Ax \in \mathbf{R}^N$.

**Generalized Newton method**

Newton's method for the equation $\boxed{F(x)=0}$:

$$x_{n+1} = x_n - (DF(x_n))^{-1} F(x_n) \quad (n = 0,1,2,\ldots)$$

This means that: $x_{n+1} = x_n - w_n \quad (n = 0,1,2,\ldots)$
where the correction term $w_n$ is the solution of the following **linear** equation:

$$DF(x_n) w_n = F(x_n)$$

If $F$ is twice continuously differentiable, $F$ has a root in $X$, and $DF(x^*)$ is *regular* (i.e. invertible with a bounded inverse), then Newton's method quadratically converges to the exact solution $x^*$ provided that the initial approximation $x_0$ is sufficiently close to $x^*$. That is, the following estimation is valid (with a proper constant $C > 0$):

$$\| x_{n+1} - x^* \| \le C \cdot \| x_n - x^* \|^2$$

*Remark*: Newton's method converts a **nonlinear** problem to a **sequence of linear** ones.

## Generalized Newton method, an example

**Inversion of a matrix**. Let $A \in \mathbf{M}_{N\times N}$ be a regular matrix. For an arbitrary regular matrix $X \in \mathbf{M}_{N\times N}$, define the following operator:

$$F(X) := X^{-1} - A$$

Then $F : \mathbf{M}_{N\times N} \to \mathbf{M}_{N\times N}$, and the unique solution of the equation $F(X) = 0$ is: $X = A^{-1}$.

Let us apply Newton's method to the matrix equation. First, calculate the derivative of $F$:

$$F(X+H) = (X+H)^{-1} - A = (X(I + X^{-1}H))^{-1} - A = (I + X^{-1}H)^{-1}X^{-1} - A$$

If the norm of the matrix $H$ is sufficiently small, then $\| X^{-1}H \| \le \| X^{-1} \| \cdot \| H \| < 1$.
Utilizing the expression $(I-B)^{-1} = I + B + B^2 + B^3 + B^4 + \ldots$ (which is valid, if $\| B \| < 1$, and implies that $(I-B)^{-1} = I - B + O(\|B\|^2)$:

$$F(X+H) = (I + X^{-1}H)^{-1}X^{-1} - A = (I - X^{-1}H + o(H))X^{-1} - A =$$
$$= X^{-1} - X^{-1}HX^{-1} + o(H) - A = F(X) - X^{-1}HX^{-1} + o(H)$$

whence

$$DF(X)H = -X^{-1}HX^{-1} \qquad \Rightarrow \qquad DF(X)^{-1}W = -XWX$$

**Generalized Newton method, an example**

Thus, the algorithm of Newton's method is as follows:

$$X_{n+1} := X_n - (DF(x_n))^{-1}(X_n^{-1} - A) = X_n + X_n(X_n^{-1} - A)X_n = \\ = X_n(2I - AX_n).$$

For the error of the approximation: $\| A^{-1} - X_n \| = \| A^{-1}(I - AX_n) \| \le \| A^{-1} \| \cdot \| I - AX_n \|$. Observe that $\| I - AX_n \|$ converges to 0 *very rapidly* (provided that the initial approximation was good enough), since:

$$I - AX_{n+1} = I - AX_n(2I - AX_n) = I - 2AX_n + AX_nAX_n = (I - AX_n)^2,$$

whence

$$\| I - AX_{n+1} \| \le \| I - AX_n \|^2$$