COURSE 11

5. Numerical methods for solving nonlinear equations in $\mathbb{R}$ (continuation)

Let $f : \Omega \to \mathbb{R}$, $\Omega \subset \mathbb{R}$. Consider the equation $f(x) = 0, \quad x \in \Omega$.

5.1. One-step methods

Let F be a one-step method, i.e., for a given x_i we have $x_{i+1} = F(x_i)$.

Another way for obtaining Newton's method.

We start with x_0 as an initial guess, sufficiently close to the α. Next approximation x_1 is the point at which the tangent line to f at $(x_0, f(x_0))$ crosses the Ox-axis. The value x_1 is much closer to the root α than x_0.

We write the equation of the tangent line at $(x_0, f(x_0))$:

$$y - f(x_0) = f'(x_0)(x - x_0).$$

If $x = x_1$ is the point where this line intersects the Ox-axis, then $y = 0$

$$-f(x_0) = f'(x_0)(x_1 - x_0),$$

and solving for x_1 gives

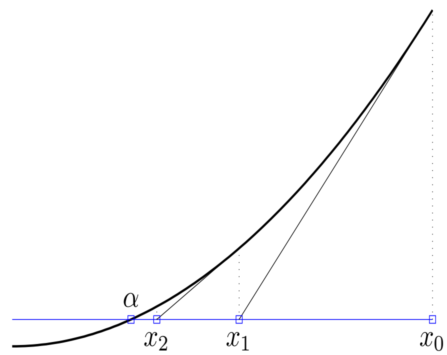
$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

By repeating the process using the tangent line at $(x_1, f(x_1))$, we obtain for x_2

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

For the general case we have

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \;\; n \geq 0. \tag{1}$$



The algorithm:

Let x_0 be the initial approximation.

for $n = 0, 1, ..., ITMAX$

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

A stopping criterion is:

$$|f(x_n)| \leq \varepsilon \text{ or } \left|x_{n+1} - x_n\right| \leq \varepsilon \text{ or } \frac{\left|x_{n+1} - x_n\right|}{\left|x_{n+1}\right|} \leq \varepsilon,$$

where ε is a specified tolerance value.

Example 1 *Use Newton's method to compute a root of* $x^3 - x^2 - 1 = 0$, *to an accuracy of* 10^{-4}. *Use* $x_0 = 1$.

Sol. *The derivative of f is* $f'(x) = 3x^2 - 2x$. *Using* $x_0 = 1$ *gives* $f(1) = -1$ *and* $f'(1) = 1$ *and so the first Newton's iterate is*

$$x_1 = 1 - \frac{-1}{1} = 2 \text{ and } f(2) = 3,\ f'(2) = 8.$$

The next iterate is

$$x_2 = 2 - \frac{3}{8} = 1.625.$$

Continuing in this manner we obtain the sequence of approximations which converges to 1.465571.

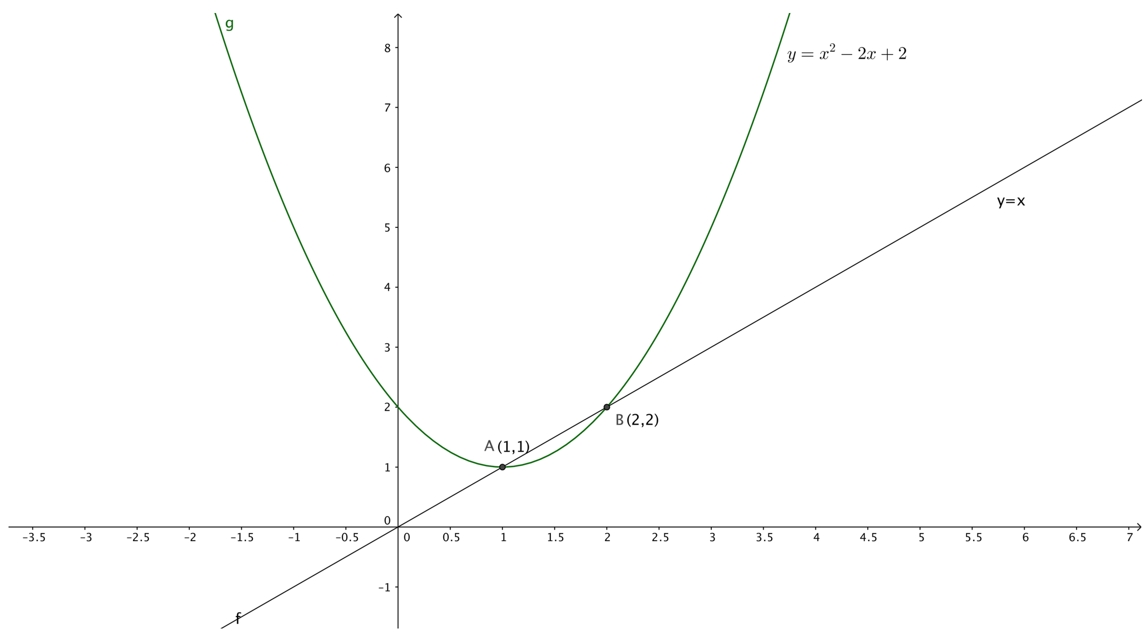
5.1.2. Fixed point iteration method (successive approximation method)

Definition 2 *The number* α *is called* **a fixed point** *of the function* $g : D \subseteq \mathbb{R} \to D$ *if* $g(\alpha) = \alpha$.

Example 3 *Find the fixed points of the function* $g(x) = x^2 - 2x + 2$.

Sol. A fixed point α of g has the property $\alpha = g(\alpha) = \alpha^2 - 2\alpha + 2$, so $0 = \alpha^2 - 3\alpha + 2 = (\alpha - 1)(\alpha - 2)$. Whence, the fixed points of g are $\alpha_1 = 1$ and $\alpha_2 = 2$.

Geometrically, the fixed points are the intersection points of the graph of the function g and the first bisection line ($y = x$). (See the following figure.)



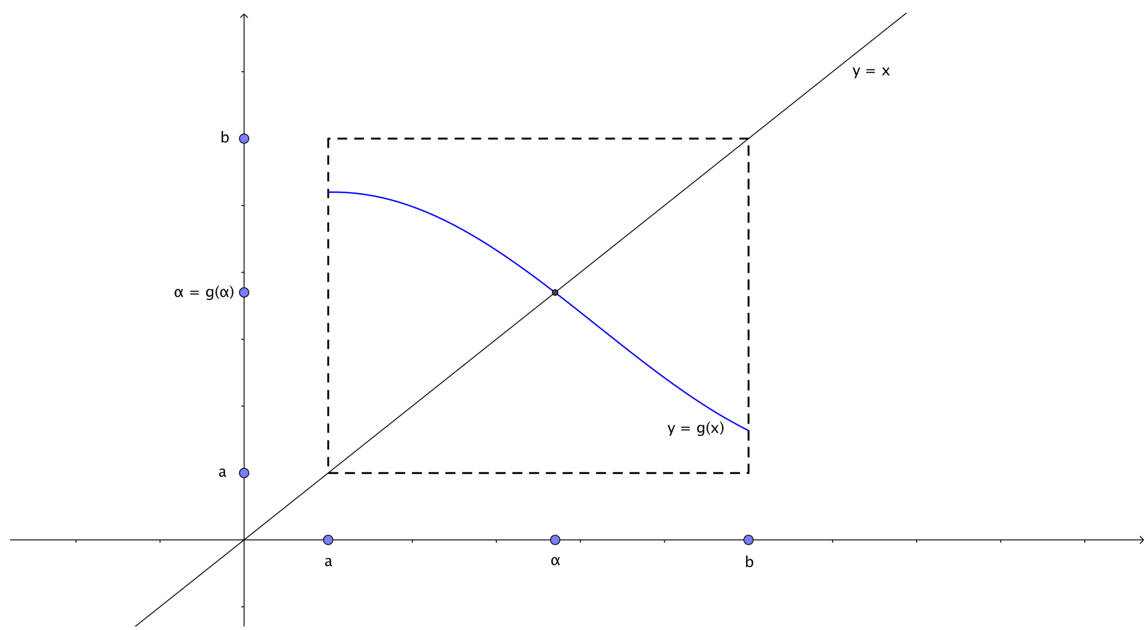
Sufficient condition for the existence and uniqueness of a fixed point:

Theorem 4 *1. If $g \in C[a,b]$ and $g(x) \in [a,b]$ for any $x \in [a,b]$, then g has at least one fixed point in $[a,b]$. In fewer words, if $g : [a,b] \to [a,b]$ and $g \in C[a,b]$ then $\exists \alpha \in [a,b]$ fixed point.*

2. Moreover, if there exists $g'(x)$ in (a,b) and

$$|g'(x)| < 1, \quad \forall x \in (a,b),$$

then the fixed point is unique in $[a,b]$.



Example 5 *Prove that* $g(x) = (x^2 - 4)/5$ *has a unique fixed point in* $[-2, 2]$.

Sol. The minimum and maximum of $g(x)$ for $x \in [-2, 2]$ are the limits of the interval, or at the points where $g'(x) = 0$. We have $g'(x) = 2x/5$, g is continuous and there exists $g'(x)$ in $[-2, 2]$. So, the minimum and maximum of $g(x)$ on $[-2, 2]$ are at $x = -2$, $x = 0$ or $x = 2$. We have $g(-2) = 0$, $g(2) = 0$, $g(0) = -4/5$, so $x = -2$ and $x = 2$ are points of absolute maximum and $x = 0$ is a point of absolute minimum in $[-2, 2]$. Moreover,

$$|g'(x)| = \left|\frac{2x}{5}\right| \leq \left|\frac{4}{5}\right| < 1, \quad \forall x \in (-2, 2).$$

So, g satisfies the conditions of Theorem 4, so it follows that g has a unique fixed point in $[-2, 2]$.

Consider the equation

$$f(x) = 0, \tag{2}$$

where $f : [a, b] \to \mathbb{R}$. Assume that $\alpha \in [a, b]$ is a zero of $f(x)$.

In order to compute α, we transform (2) algebraically into *fixed point form*,

$$x = g(x), \tag{3}$$

where g is chosen so that $g(x) = x \Leftrightarrow f(x) = 0$.

A simple way to do this is, for example, $x = x + f(x) =: g(x)$.

Finding a zero of $f(x)$ in $[a, b]$ is then equivalent to finding a fixed point $x = g(x)$ in [a, b].

The fixed point form suggests *the fixed point iteration*

$$x_0 - \text{initial guess}, x_{k+1} = g(x_k),\ \ k = 0, 1, 2, \ldots.$$

The hope is that iteration will produce a convergent sequence $(x_n) \to \alpha$.

For example, consider

$$f(x) = xe^x - 1 = 0. \tag{4}$$

A first fixed point iteration is obtained rearranging and dividing (4) by e^x: $xe^x = 1 \Rightarrow x = e^{-x}$, so $x = g(x) = e^{-x}$ and

$$x_{k+1} = e^{-x_k}.$$

With the initial guess $x_0 = 0.5$ we obtain the iterates $x_1 = 0.6065306597$, $x_2 = 0.5452392119, ..., x_8 = 0.5664094527, x_9 = 0.5675596343, ...,$ $x_{28} = 0.56714328, x_{29} = 0.56714329$

So x_k seems to converge to $\alpha = 0.5671432...$

A second fixed point form is obtained from $xe^x = 1$ by adding x on both sides: $xe^x + x = 1 + x \Rightarrow x(e^x + 1) = 1 + x \Rightarrow x = \frac{1+x}{e^x+1}$, we get

$$x = g(x) = \frac{1 + x}{e^x + 1}.$$

This time the convergence is much faster (we need only three iterations to obtain a 10-digit approximation of α) : $x_0 = 0.5$, $x_1 = 0.5663110032$, $x_2 = 0.5671431650$, $x_3 = 0.5671432904$.

Another possibility for a fixed point iteration is $x = x + 1 - xe^x$. But this iteration function does not generate a convergent sequence.

Finally we could also consider the fixed point form $x = x + xe^x - 1$. Also this iteration function does not generate a convergent sequence.

The question is: when does the iteration sequence converge?

Answer: when conditions of Theorem 4 are fulfilled.

For this example, we have two cases when $|g'(x)| < 1$ and the algorithm converges and two cases when $|g'(x)| > 1$ and the algorithm is not convergent.

A more general statement for the convergence is the theorem of Banach.

Definition 6 **A Banach space** *$\mathcal{B}$ is a complete normed vector space over some number field K such as $\mathbb{R}$ or $\mathbb{C}$.* (Complete *means that every Cauchy sequence converges in $\mathcal{B}$.)*

Definition 7 *Let $A \subset \mathcal{B}$ be a closed subset and $G : A \to A$. G is called* **Lipschitz continuous** *on A if there exists a constant $L \geq 0$ such that $||G(x) - G(y)|| \leq L\, ||x - y||$, $\forall x, y \in A$. Furthermore, G is called* **a contraction** *if L can be chosen such that $L < 1$.*

Theorem 8 *(Banach Fixed Point Theorem) Let A be a closed subset of a Banach space $\mathcal{B}$, and let G be* **a contraction** *$G : A \to A$. Then:*

a) G has a unique fixed point α, which is the unique solution of the equation $x = G(x)$.

b) The sequence $x_{n+1} = G(x_n)$ *converges to* α *for every initial guess* $x_0 \in A$.

c) We have the estimate: $||\alpha - x_n|| \leq \frac{L^{n-l}}{1-L}||x_{l+1} - x_l||$, *for* $0 \leq l \leq n$ *(or* $||\alpha - x_n|| \leq \frac{L^n}{1-L}||x_1 - x_0||$)

For practical applications is also useful the following estimation.

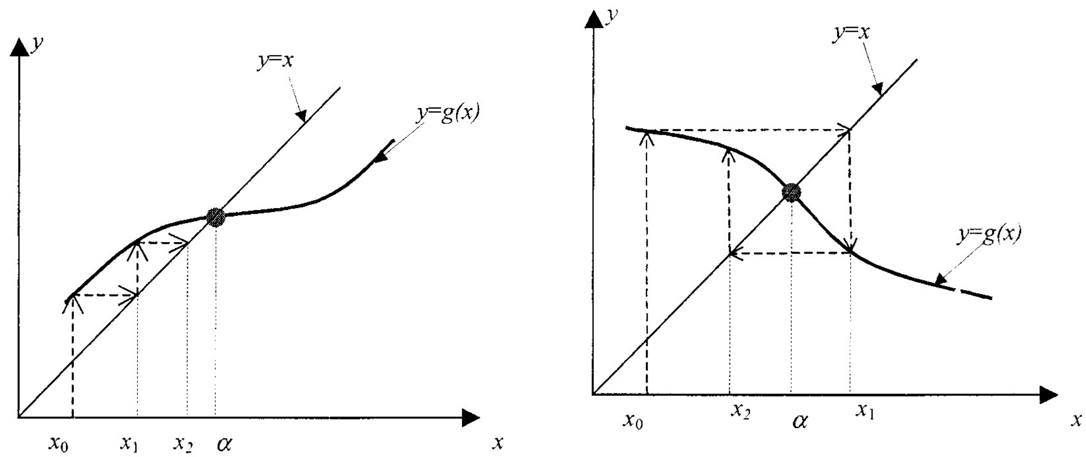
Lemma 9 *If* $\|G'(x)\| < L < 1$, $x \in V(\alpha)$ *then*

$$||\alpha - x_n|| \leq \frac{L}{1-L}||x_n - x_{n-1}||.$$

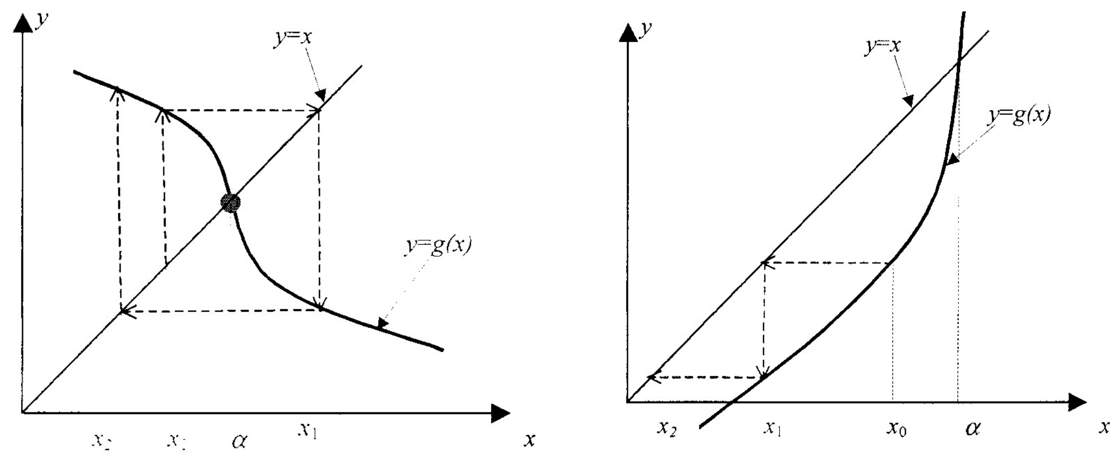
Geometric interpretation of the method: we plot $y = G(x)$ and $y = x$. The intersection points of the two functions are the solutions of $x = G(x)$. The computation of the sequence $\{x_k\}$ with x_0 chosen initial value, $x_{k+1} = G(x_k), k = 0, 1, 2, ...$ can be interpreted geometrically via sequences of lines parallel to the coordinate axes:

x_0	start with x_0 on the x-axis
$G(x_0)$	go parallel to the y-axis to the graph of G
$x_1 = G(x_0)$	move parallel to the x-axis to the graph $y = x$
$G(x_1)$	go parallel to the y-axis to the graph of G
etc.	

Case of convergence $|G'(x)| < 1$.



Case of divergence $|G'(x)| > 1$.



When $|g'(\alpha)| = 1$, depending on the mapping g, the iterates may converge or not (e.g., $g(x) = x - x^3$ or $g(x) = x + x^3$).

5.2. Multistep methods

Lagrange inverse interpolation

Let $y_k = f(x_k)$, $k = 0, ..., n$, hence $x_k = g(y_k)$. We attach the Lagrange interpolation formula to y_k and $g(y_k)$, $k = 0, ..., n$:

$$g = L_n g + R_n g, \tag{5}$$

where

$$(L_n g)(y) = \sum_{k=0}^{n} \frac{(y-y_0)...(y-y_{k-1})(y-y_{k+1})...(y-y_n)}{(y_k-y_0)...(y_k-y_{k-1})(y_k-y_{k+1})...(y_k-y_n)} g(y_k). \tag{6}$$

Taking

$$F_n^L(x_0, ..., x_n) = (L_n g)(0),$$

F_n^L is a $(n+1)-$ steps method defined by

$$F_n^L(x_0,...,x_n) = \sum_{k=0}^{n} \frac{y_0 \cdots y_{k-1} y_{k+1} \cdots y_n}{(y_k - y_0) \ldots (y_k - y_{k-1})(y_k - y_{k+1}) \ldots (y_k - y_n)} (-1)^n g(y_k)$$
$$= \sum_{k=0}^{n} \frac{y_0 \cdots y_{k-1} y_{k+1} \cdots y_n}{(y_k - y_0) \ldots (y_k - y_{k-1})(y_k - y_{k+1}) \ldots (y_k - y_n)} (-1)^n x_k.$$

Concerning the convergence of this method we state:

Theorem 10 *If $\alpha \in (a,b)$ is solution of equation $f(x) = 0$, f' is bounded on (a,b), and the starting values satisfy $|\alpha - x_k| < 1/c$, $\quad k = 0,...,n$, with $c =$constant, then the sequence*

$$x_{i+1} = F_n^L(x_{n-i},...,x_i), \quad i = n, n+1, ...$$

converges to α.

Remark 11 *The order $ord(F_n^L)$ is the positive solution of the equation*

$$t^{n+1} - t^n - ... - t - 1 = 0.$$

Particular cases.

1) For $n = 1$, the nodes x_0, x_1, we get **the secant method**

$$F_1^L(x_0, x_1) = x_1 - \frac{(x_1 - x_0) f(x_1)}{f(x_1) - f(x_0)},$$

Thus,

$$x_{k+1} := F_1^L(x_{k-1}, x_k) = x_k - \frac{(x_k - x_{k-1}) f(x_k)}{f(x_k) - f(x_{k-1})}, \qquad k = 1, 2, ...$$

is the new approximation obtained using the previous approximations x_{k-1}, x_k.

The *order* of this method is the positive solution of equation:

$$t^2 - t - 1 = 0,$$

so $ord(F_1^L) = \frac{(1+\sqrt{5})}{2} \approx 1.618$. (the Golden Ratio ($\phi$)). (Two numbers a, b are in Golden Ratio if $\frac{a+b}{a} = \frac{a}{b} = \phi$)

A modified form of the secant method: if we keep x_1 fixed and we change every time the same interpolation node, i.e.,

$$x_{k+1} = x_k - \frac{(x_k - x_1) f(x_k)}{f(x_k) - f(x_1)}, \quad k = 2, 3, \ldots.$$

2) For $n = 2$, the nodes x_0, x_1, x_2 and we get

$$F_2^L(x_0, x_1, x_2) = \frac{x_0 f(x_1) f(x_2)}{[f(x_0) - f(x_1)][f(x_0) - f(x_2)]} + \frac{x_1 f(x_0) f(x_2)}{[f(x_1) - f(x_0)][f(x_1) - f(x_2)]} + \frac{x_2 f(x_0) f(x_1)}{[f(x_2) - f(x_0)][f(x_2) - f(x_1)]}.$$

The *order* of this method is the positive solution of equation:

$$t^3 - t^2 - t - 1 = 0,$$

so $ord(F_2^L) = 1.8394$.

Comparing the Newton's method and secant method with respect to the time needed for finding a root with some given precision, we have:

-Newton's method has more computation at one step: it is necessary to evaluate $f(x)$ and $f'(x)$. Secant method evaluates just $f(x)$ (supposing that $f(x_{previous})$ is stored.)

-The number of iterations for Newton's method is smaller (its order is $p_N = 2$). Secant method has order $p_S = 1.618$ and we have that three steps of this method are equivalent with two steps of Newton's method.

- It is proved that if the time for computing $f'(x)$ is greater than (0.44$\times$the time for computing $f(x)$), then the secant method is faster.

Remark 12 *The computation time is not the unique criterion in choosing the method! Newton's method is easier to apply. If $f(x)$ is not explicitly known (for example, it is the solution of the numerical integration of a differential equation), then its derivative is computed numerically. If we consider the following expression for the numerical computation of derivative:*

$$f'(x) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} \tag{7}$$

then the Newton's method becomes the secant method.

Another way of obtaining secant method.

Based on approx. the function by a straight line connecting two points on the graph of f (not required f to have opposite signs at the initial points).

The first point, x_2, of the iteration is taken to be the point of intersection of the Ox-axis and the secant line connecting two starting points $(x_0, f(x_0))$ and $(x_1, f(x_1))$. The next point, x_3, is generated by the intersection of the new secant line, joining $(x_1, f(x_1))$ and $(x_2, f(x_2))$ with the Ox-axis. The new point, x_3, together with x_2, is used to generate the next point, x_4, and so on.

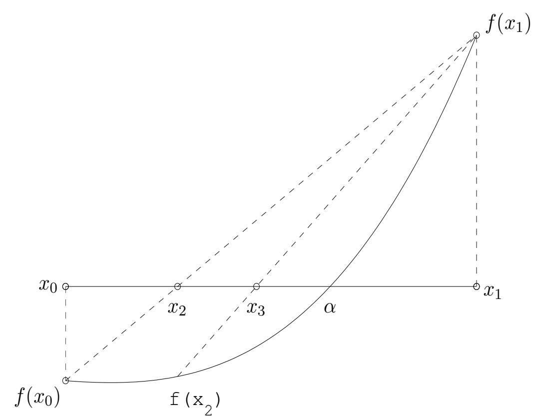
The formula for x_{n+1} is obtained by setting $x = x_{n+1}$ and $y = 0$ in the equation of the secant line from $(x_{n-1}, f(x_{n-1}))$ to $(x_n, f(x_n))$:

$$\frac{x - x_n}{x_{n-1} - x_n} = \frac{y - f(x_n)}{f(x_{n-1}) - f(x_n)} \Leftrightarrow x = x_n + \frac{(x_{n-1} - x_n)(y - f(x_n))}{f(x_{n-1}) - f(x_n)},$$

we get

$$x_{n+1} = x_n - f(x_n)\left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}\right]. \tag{8}$$

Note that x_{n+1} depends on the two previous elements of the sequence $\Rightarrow$ two initial guesses, x_0 and x_1,for generating $x_2, x_3, \ldots$.



The algorithm:

Let x_0 and x_1 be two initial approximations.

for $n = 1, 2, ..., ITMAX$

$$x_{n+1} \leftarrow x_n - f(x_n)\left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}\right].$$

A suitable stopping criterion is

$$|f(x_n)| \leq \varepsilon \text{ or } \left|x_{n+1} - x_n\right| \leq \varepsilon \text{ or } \frac{\left|x_{n+1} - x_n\right|}{\left|x_{n+1}\right|} \leq \varepsilon,$$

where ε is a specified tolerance value.

Example 13 *Use the secant method with* $x_0 = 1$ *and* $x_1 = 2$ *to solve* $x^3 - x^2 - 1 = 0$, *with* $\varepsilon = 10^{-4}$.

Sol. *With* $x_0 = 1$, $f(x_0) = -1$ *and* $x_1 = 2$, $f(x_1) = 3$, *we have*

$$x_2 = 2 - \frac{(2-1)(3)}{3-(-1)} = 1.25$$

from which $f(x_2) = f(1.25) = -0.609375$. *The next iterate is*

$$x_3 = 1.25 - \frac{(1.25-2)(-0.609375)}{-0.609375-3} = 1.3766234.$$

Continuing in this manner the iterations lead to the approximation 1.4655713.