PROGRAM ROZWOJOWY
POLITECHNIKI WARSZAWSKIEJ

LECTURE 4

BASIC METHODS FOR NONLINEAR ALGEBRAIC EQUATIONS

KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

UNIA EUROPEJSKA
EUROPEJSKI
FUNDUSZ SPOŁECZNY

In this lecture, we discuss the problem how to find numerically the approximate solution to the nonlinear algebraic equation

$$f(x) = 0$$

In the above, the symbol f refers to a given function. Usually, such equation cannot be solved analytically. Consider for instance

$$x^5 - x^2 + 4x - 1 = 0$$

$$e^{-x} + \sin(x) = 0$$

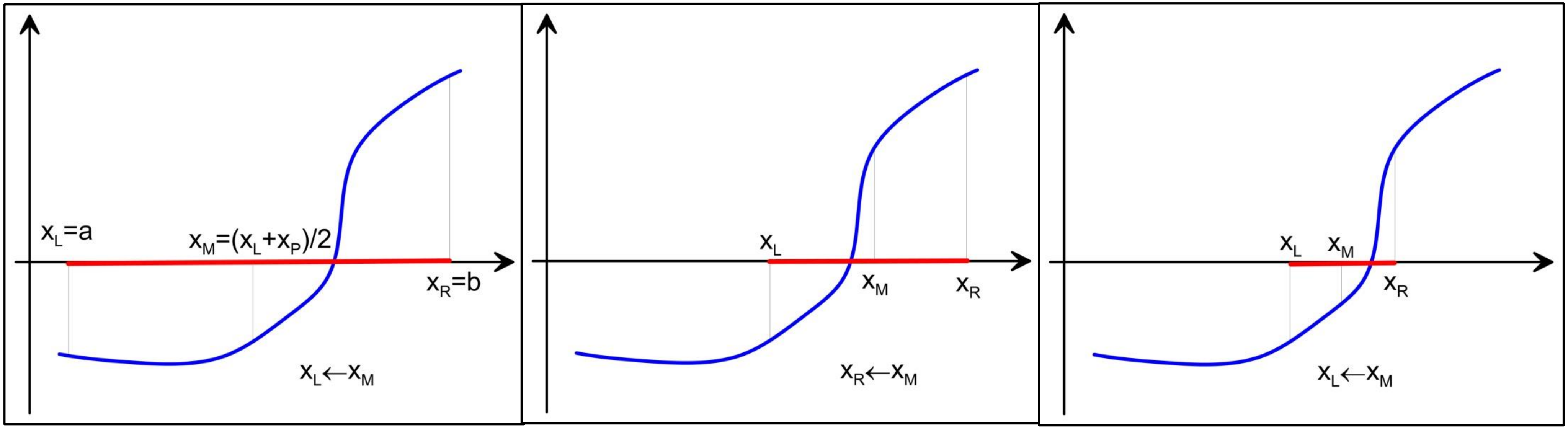
$$4 - x - \tan^{-1}(x) = 0$$

The only possibility is to find an approximate value of the solution (the root of f) by means of some iterative calculations. In this lecture we present a number of the most elementary approaches to this problem.

Note: in the CS2 course we consider only the case of a **single equation**. The algorithms for the nonlinear algebraic systems of equations will be covered by more advanced courses of numerical methods.

THE BISECTION METHOD

Let's begin with the method of bisection. It is very elementary approach. Its "mechanics" is explained graphically in the figures below



Once the interval containing the root has been found, it is subsequently halved and the half containing the root is recognized. The identification of the proper half is based on the assessment of the sign of the function values at the endpoints of the current subinterval.

Since the function is assumed continuous, the presence of the root is guaranteed in the subinterval with opposite-sign endpoint values of the function.

Pseudo code of the bisection method is shown below

$$
\begin{array}{l}
START : f_L := f(x_L) \quad ; \quad f_R := f(x_R) \\
if \;\; (f_L \cdot f_R < 0) \; then \\
\quad while \; (x_R - x_L > 2\varepsilon) \; do \\
\qquad x_M := (x_R + x_L)/2 \\
\qquad f_M := f(x_M) \\
\qquad if \;\; (f_L \cdot f_M < 0) \; then \\
\qquad\quad x_R := x_M \; ; \; f_R := f_M \\
\qquad else \\
\qquad\quad x_L := x_M \; ; \; f_L := f_M \\
\qquad endif \\
\quad enddo \\
\quad return(x_M) \\
else \\
\quad change \; the \; interval \; [x_L, x_R]; \\
\quad return \; to \; START; \\
endif
\end{array}
$$

Assume we want to determine the root x_* with the absolute error ε, i.e., we will terminate the bisection process as soon as

$$\left|x_* - x_M\right| \le \varepsilon$$

Note that after n steps of the process we have the estimate

$$\left|x_* - x_M\right| \le \frac{b-a}{2^n}$$

Thus, the number of steps which guarantees achieving a desirable accuracy is

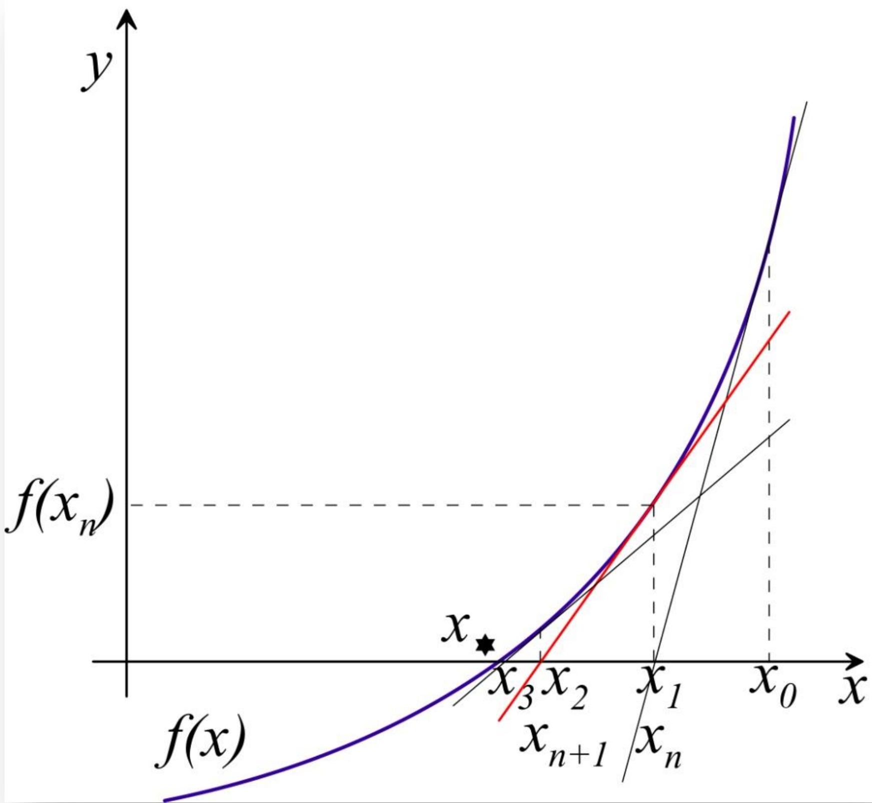
$$n \ge \log_2 \frac{b-a}{\varepsilon}$$

Bisection method – pros and cons

Pros: if the initial interval is property chosen then the bisection method will always converge to the root (some root) of the continuous function *f*

Cons: the method is essentially insensitive to the local shape of the function (like the slope) and usually converges rather slowly (requires many evaluation of the function *f*, which can be very costly).

METHOD OF TANGENTS (THE NEWTON'S METHOD)



The Newton's method is a very efficient method of finding roots of the sufficiently smooth functions. The idea of this method is explained graphically in the figure below.

Thus, the next approximation to the root x_* is defined as the abscissa of the point of intersection between x-axis and the line tangent to the plot of the function f.

The equation of the tangent line reads

$$y = f'(x_n)(x - x_n) + f(x_n)$$

Then, from the equation

$$0 = f'(x_n)(x_{n+1} - x_n) + f(x_n)$$

we obtain

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

We will show that the method of tangents exhibits (under some conditions) a **quadratic convergence**. To this aim, we apply the Taylor expansion formula and write

$$f(x_*) = f(x_n) + f'(x_n)(x_* - x_n) + \tfrac{1}{2} f''(\xi)(x_* - x_n)^2$$

In the above, $\xi \in [\min(x_n, x_*), \max(x_n, x_*)]$. Next, since $f(x_*) \equiv 0$ one obtains

$$\begin{aligned} 0 &= f(x_n) + f'(x_n)(x_* - x_n) + \tfrac{1}{2} f''(\xi)(x_* - x_n)^2 = \\ &= f(x_n) - f'(x_n)x_n + f'(x_n)x_* + \tfrac{1}{2} f''(\xi)(x_* - x_n)^2 = \\ &= -f'(x_n)\underbrace{\left(x_n - \frac{f(x_n)}{f'(x_n)}\right)}_{x_{n+1}} + f'(x_n)x_* + \tfrac{1}{2} f''(\xi)(x_* - x_n)^2 = \\ &= f'(x_n)(x_* - x_{n+1}) + \tfrac{1}{2} f''(\xi)(x_* - x_n)^2 \end{aligned}$$

Thus, we conclude that $$\left|x_* - x_{n+1}\right| = \left|\frac{f''(\xi)}{2 f'(x_n)}\right| \left|x_* - x_n\right|^2$$

The following **local convergence theorem** can be now formulated:

Assume that for the certain interval $I_\alpha = (x_* - \alpha, x_* + \alpha)$ the following conditions hold:

$$1)\ \underset{M>0}{\exists}\ \underset{x\in I_\alpha}{\forall}\ \left|f''(x)\right| \le M$$

$$2)\ \underset{m>0}{\exists}\ \underset{x\in I_\alpha}{\forall}\ \left|f'(x)\right| \ge m$$

Then for each $x_0 \in I_\alpha$ and such that $\frac{M}{2m}\left|x_* - x_0\right| \le \gamma < 1$ the following estimate is valid

$$\left|x_* - x_1\right| \le \frac{M}{2m}\left|x_* - x_0\right|^2 \le \gamma\left|x_* - x_0\right|$$

which leads to the conclusion that $x_1 \in I_\alpha$ and by the induction argument

$$\left|x_* - x_{n+1}\right| \le \gamma\left|x_* - x_n\right| \le \gamma^{n+1}\left|x_* - x_n\right|$$

Thus $\left|x_* - x_n\right| \xrightarrow[n\to\infty]{} 0$ (so we have convergence). Moreover $\left|x_* - x_{n+1}\right| \le \frac{M}{2m}\left|x_* - x_n\right|^2$

REMARK: Note that the above theorem provides condition which guarantee the **local convergence** only. In other words, the Newton's method will "typically" achieve the quadratic convergence rate providing that it is already **sufficiently close to the solution**. On the other hand, if the initial point x_0 is not sufficiently close to x_* then the Newton's iterations will not converge to this root (and perhaps they will diverge to infinity).

What if other assumptions do not hold? Consider the following counterexample:

$$f(x) = x^2 - 2x + 1 = 0 \quad \Rightarrow \quad x_* = 1$$

Then $f'(x) = 2x - 2$, $f'(1) = 0$, and we have

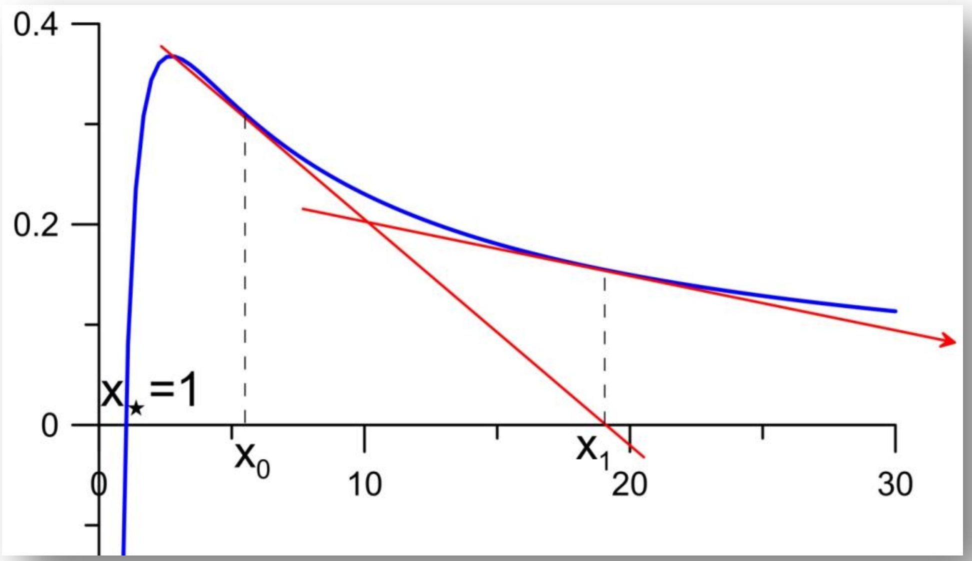
$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{(x_n - 1)^2}{2(x_n - 1)} = x_n - \tfrac{1}{2}(x_n - 1) = \tfrac{1}{2}x_n + \tfrac{1}{2}$$

Eventually, $x_{n+1} - 1 = \tfrac{1}{2}(x_n - 1)$ which shows that the distance from the root shrinks linearly (by the factor of ½) during the process. The Newton's method fails to achieve quadratic convergence because the $f'(x_*) = 0$.

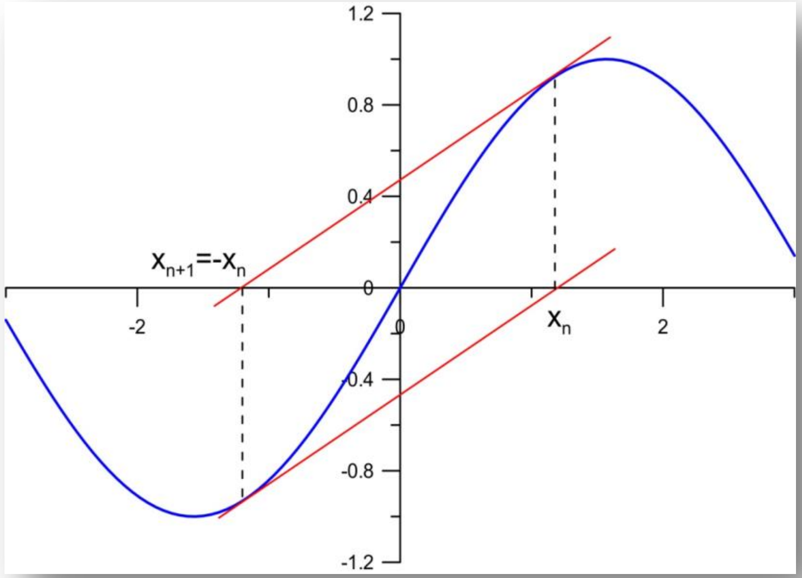
More examples (exercises for the Reader)

1. Show that if $f(x)=(x-a)^m$ then the Newton's method generation then $x_{n+1}-a=(1-\frac{1}{m})(x_n-a)$. Note that for large m the convergence can be pretty slow!
2. Analyze the convergence rate (to the zero solution) of the Newton's method applied to the equation $x^{3/2}+2x=0$

Consider some other examples which demonstrate the possible "pathological" behavior of the Newton's method.



Example 1: The region of local convergence can be pretty narrow like for the function $f(x)=\ln(x)/x$ with $x_*=1$. It can be clearly seen from the figure below that the choice of any starting point located on the right-hand side of the function's maximum leads to divergence to infinity. On the other hand, point located on the left-hand side but to close to minimum will yield the next approximation beyond the domain of the function (which is R_+)



Example 2: The iterations of the Newton's method can loop in a cycle. An example (rather artificial) of such behavior is provided by the function

$$f(x) = \sin(x)$$

Imagine, we start the iterations from the initial point x_0 such that

$$x_0 = \tfrac{1}{2}\tan(x_0)$$

Then

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

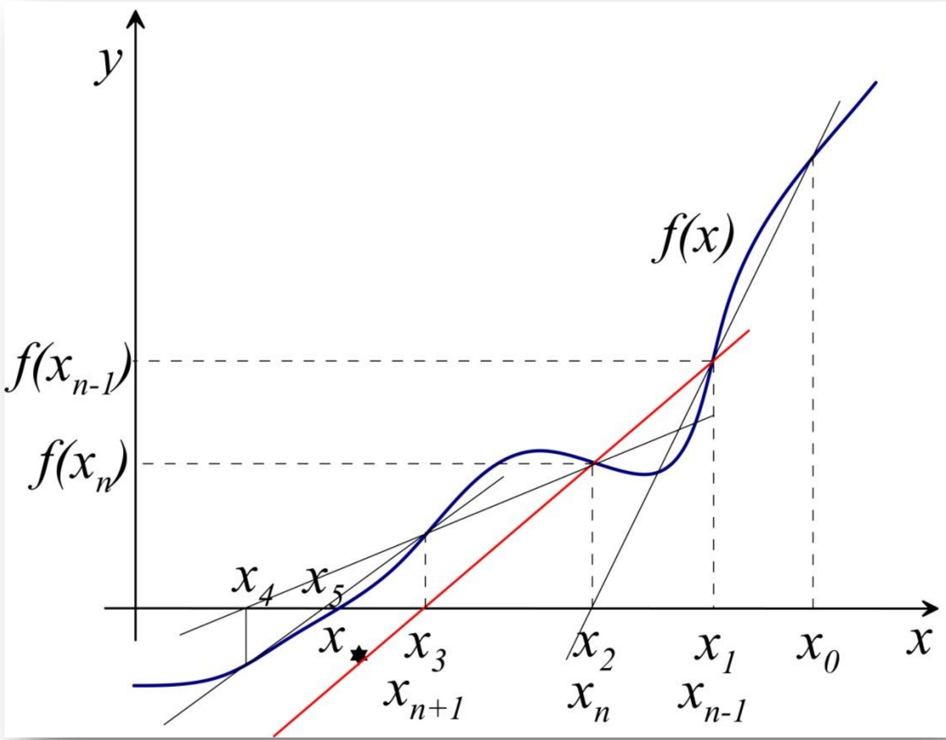
$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = -x_0 - \frac{\sin(-x_0)}{\cos(-x_0)} = -x_0 + \tan(x_0) = x_0$$

So – at least theoretically – the iterations cycle forever between two values: x_0 and $-x_0$.

Problem: In reality computers always make approximations (the computer arithmetic is not exact). What is the sensitivity of the above cycling behavior to small (and inevitable) perturbation of the data? Perform such analysis analytically (not trivial) or by the computer experiment.

METHOD OF SECANTS

The possibly weak point of the Newton's method is that it requires to compute the value(s) of the 1st derivative. This may pose a problem, especially when the explicit formula for the function f is not available. This difficulty is surpassed by the method of secants. The "mechanics" of this method is explained in the figure.



This time, the next approximation x_{n+1} to the root x_* is defined as the abscissa of the point of intersection between x-axis and the secant line passing through the points $(x_{n-1}, f(x_{n-1}))$ and $(x_n, f(x_n))$.

The equation of this line is

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

Thus, one obtain the formula of the **method of secants**

$$0 = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}(x_{n+1} - x_n) + f(x_n)$$

$$\Downarrow$$

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

We will analyze the **convergence** of the method of secants. Using the Taylor expansion theorem, we write

$$f(x_n) = f(x_*) + f'(x_*)\varepsilon_n + \tfrac{1}{2} f''(x_*)\varepsilon_n^2 + \ldots$$

$$f(x_{n-1}) = f(x_*) + f'(x_*)\varepsilon_{n-1} + \tfrac{1}{2} f''(x_*)\varepsilon_{n-1}^2 + \ldots$$

The triple-dot symbol indicated that all higher-order terms (H.O.T.) follows.

The further calculation proceeds as follows:

$$\varepsilon_{n+1} = x_{n+1} - x_* = \underbrace{x_n - x_*}_{\varepsilon_n} - \frac{f(x_n)}{f(x_n) - f(x_{n-1})}[\underbrace{x_n - x_*}_{\varepsilon_n} - (\underbrace{x_{n-1} - x_*}_{\varepsilon_{n-1}})] =$$

$$= \varepsilon_n - \frac{[f'(x_*)\varepsilon_n + \tfrac{1}{2} f''(x_*)\varepsilon_n^2 + \ldots](\varepsilon_n - \varepsilon_{n-1})}{f'(x_*)\varepsilon_n + \tfrac{1}{2} f''(x_*)\varepsilon_n^2 + \ldots - [f'(x_*)\varepsilon_{n-1} + \tfrac{1}{2} f''(x_*)\varepsilon_{n-1}^2 + \ldots]} =$$

$$= \varepsilon_n - \frac{f'(x_*)\varepsilon_n + \tfrac{1}{2} f''(x_*)\varepsilon_n^2 + \ldots}{f'(x_*) + \tfrac{1}{2} f''(x_*)(\varepsilon_{n-1} + \varepsilon_n) + \ldots} = \varepsilon_n - \frac{\varepsilon_n + \tfrac{1}{2}\frac{f''(x_*)}{f'(x_*)}\varepsilon_n^2 + \ldots}{1 + \tfrac{1}{2}\frac{f''(x_*)}{f'(x_*)}(\varepsilon_{n-1} + \varepsilon_n) + \ldots} =$$

$$= \varepsilon_n - \left(\varepsilon_n + \tfrac{1}{2}\frac{f''(x_*)}{f'(x_*)}\varepsilon_n^2 + \ldots\right) \cdot \left(1 - \tfrac{1}{2}\frac{f''(x_*)}{f'(x_*)}(\varepsilon_{n-1} + \varepsilon_n) + \ldots\right) =$$

$$= \tfrac{1}{2}\frac{f''(x_*)}{f'(x_*)}(\varepsilon_{n-1} + \varepsilon_n)\varepsilon_n - \tfrac{1}{2}\frac{f''(x_*)}{f'(x_*)}\varepsilon_n^2 + \ldots = \tfrac{1}{2}\frac{f''(x_*)}{f'(x_*)}\varepsilon_{n-1}\varepsilon_n + H.O.T.$$

Hence, we have arrived at the asymptotic formula

$$\varepsilon_{n+1} \cong \frac{f''(x_*)}{2f'(x_*)}\varepsilon_n\varepsilon_{n-1} = K\varepsilon_n\varepsilon_{n-1}$$

We would like to derive an explicit estimate which involves only ε_n and ε_{n+1}.

To this aim, we anticipate the final form of this estimate as $\varepsilon_{n+1} = K^{\beta}\varepsilon_n^{\alpha}$.

It follows that $\varepsilon_n = K^{\beta}\varepsilon_{n-1}^{\alpha} \;\Rightarrow\; \varepsilon_{n-1} = K^{-\beta/\alpha}\varepsilon_n^{1/\alpha}$. After insertion, we get the alternative form, namely

$$\varepsilon_{n+1} = K\varepsilon_n\varepsilon_{n-1} = K\varepsilon_n(K^{-\beta/\alpha}\varepsilon^{1/\alpha}) = K^{1-\frac{\beta}{\alpha}}\varepsilon^{\frac{1+\alpha}{\alpha}}$$

However, both forms of the relation between ε_n and ε_{n+1} must be equivalent. Hence

$$\alpha = \frac{1+\alpha}{\alpha} \;\Rightarrow\; \alpha^2 - \alpha - 1 = 0$$

Only positive root makes sense so we finally have $\alpha = \dfrac{1+\sqrt{5}}{2} \approx 1.618$.

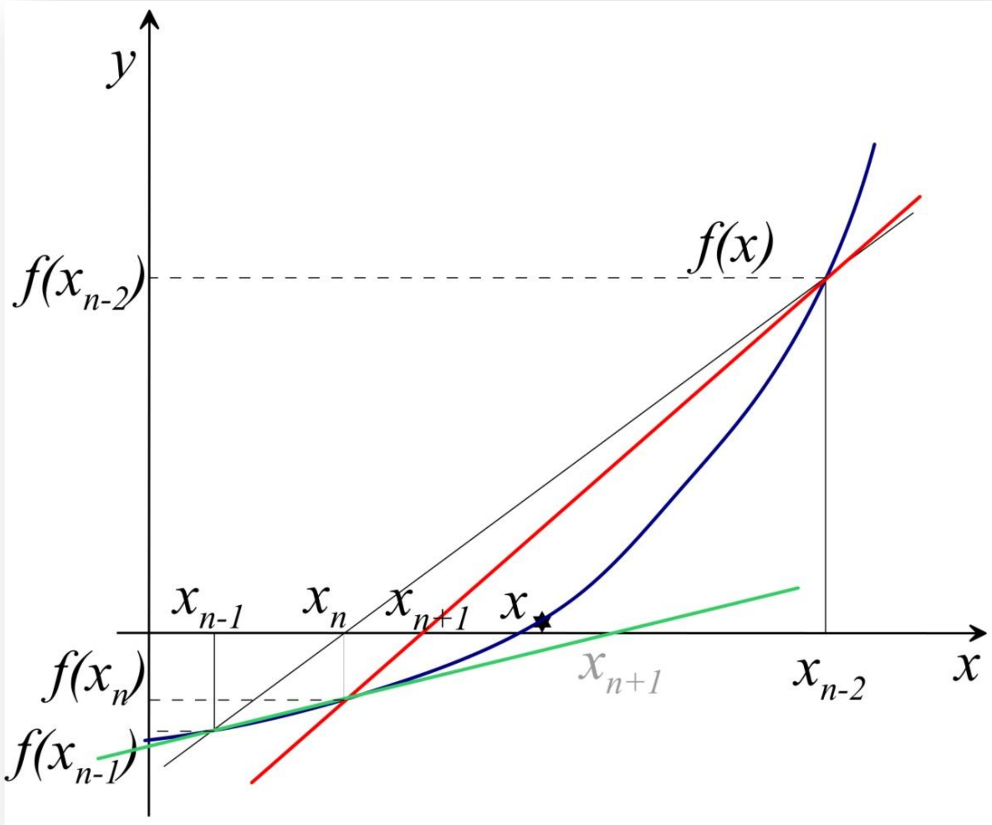
Note also that

$$\beta = 1 - \frac{\beta}{\alpha} \quad \Rightarrow \quad \beta = \frac{\alpha}{1+\alpha} = \frac{1}{\alpha}$$

Since $1 < \alpha < 2$ we say that the **convergence rate of the method of secants** is **superlinear**.

The method of secants is sensitive to "pathologies" similar to those discussed for the Newton's method. In particular, it is convergent only locally, which practically means that the initial approximation of the root must be sufficiently accurate.

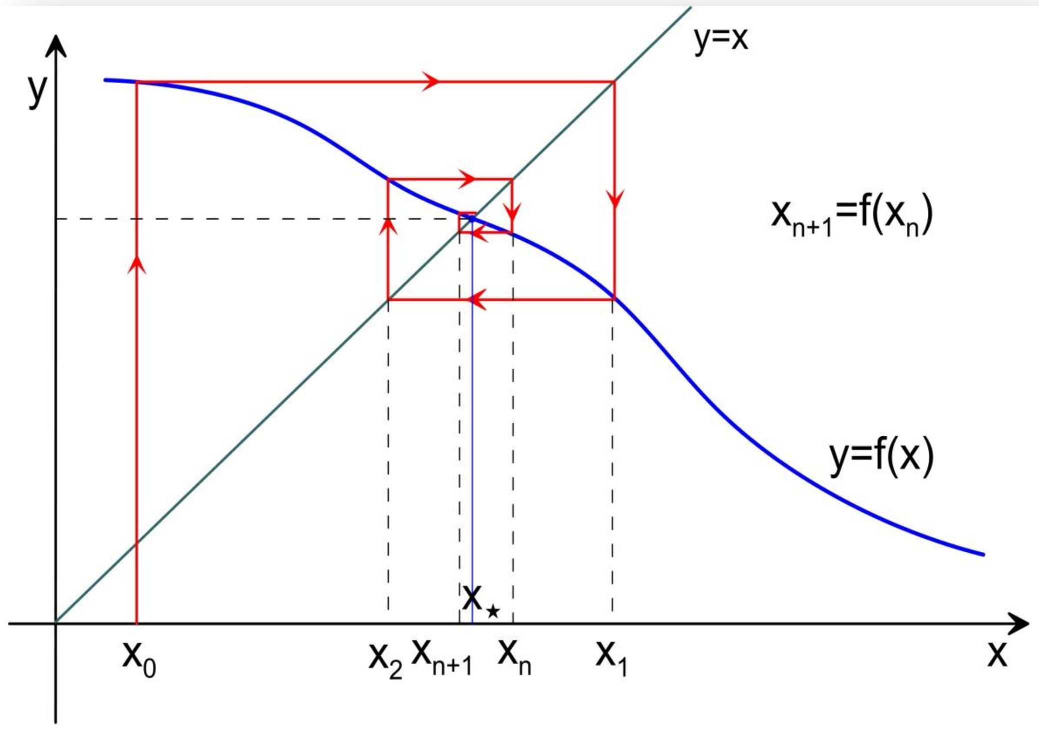
On the other hand, an interesting modification is the "false position" variant (Regula Falsi). This modification is illustrated in the following figure.



The basic difference between method of secants and the Regula Falsi consists in the following. In the case depicted in the Figure, the point x_{n+1} would be located where the green line crosses the x-axis. In the falsi rule, this point is where the red line crosses the x-axis. In other words, the secant line is spanned between two most recent points located at opposite sides of the x-axis. If two first point of the Regula Falsi iterations bracket the root then the **convergence is guaranteed**. On the other hand, the **superlinear convergence is lost**.

Yet another approach is the **method of simple iterations** which we will discuss next.

METHOD OF SIMPLE ITERATIONS



Consider the nonlinear algebraic equation in the form

$$x = g(x)$$

It natural to define the following iterative process (simple iterations)

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

Note that if this process is convergent to certain value x_* then automatically

$$x_* \equiv g(x_*)$$

In other words: **the solution is the fixed point of this iterative process**.

In the figure above, the convergence of the process is evident. Is this always the case? What is the rate of convergence? It turn out that the answers to both questions involve just one number: the value of the 1st derivative $g'(x_*)$.

To assess the rate of convergence of the simple iteration process we proceed as follows:

$$x_{n+1} = g(x_n) \;\Rightarrow\; \underbrace{x_{n+1} - x_*}_{\varepsilon_{n+1}} = g(x_n) - g(x_*) = g'(x_*)(\underbrace{x_n - x_*}_{\varepsilon_n}) + \ldots$$

Then, for sufficiently small distances from the root the following relation holds

$$\left|\varepsilon_{n+1}\right| \cong \left|g'(x_*)\right| \cdot \left|\varepsilon_n\right|$$

We immediately conclude that the root x_* **is the attracting fixed point of the simple iterations if and only if**

$$\left|g'(x_*)\right| < 1$$

Note: If the following conditions hold at the root x_*

$$\left|g'(x_*)\right| = 0 \text{ and } \left|g''(x_*)\right| < \infty$$

then the simple iteration method is **quadraticly convergent**.

Indeed:

$$x_{n+1} - x_* = g(x_n) - g(x_*) = \underset{0}{g'(x_*)}(x_n - x_*) + \tfrac{1}{2} g''(x_*)(x_n - x_*)^2 + \ldots$$

$$\Downarrow$$

$$\left|\varepsilon_{n+1}\right| \cong \tfrac{1}{2}\left|g''(x_*)\right|\left|\varepsilon_n\right|^2$$

Example: The formula of the Newton's Method can be interpreted as the simple iteration procedure for the function

$$g(x) = x - \frac{f(x)}{f'(x)}.$$

We have $$g'(x) = 1 - \frac{[f'(x)]^2 - f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2}.$$

Now, if the first derivative is not zero and the second derivative is bounded then

$$g'(x_*) = \frac{f''(x_*)}{[f'(x_*)]^2} \underbrace{f(x_*)}_{0} = 0$$

and thus the method is quadraticly convergent (as we already know).

Note: if $\left|g'(x_*)\right| \geq 1$ the method of simple iterations will typically **diverge** or it will be convergent only for specially chosen initial points (the Reader is advised to elaborate on details). It case of multiply roots, the converge to other root may also occur.