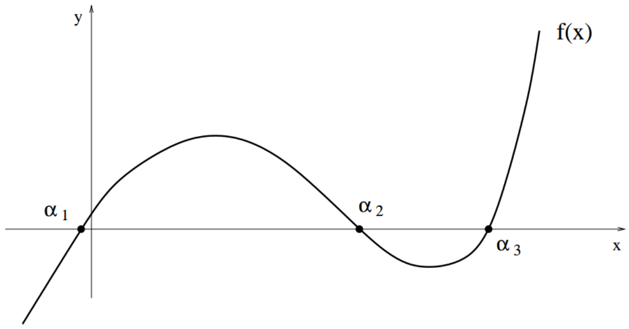
Nonlinear equations

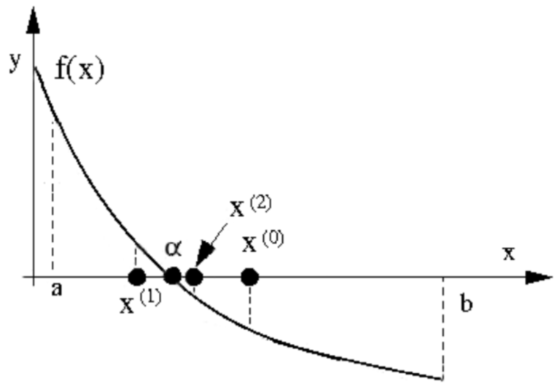
We may want to find the roots of scalar (or vector) non-linear functions, so find $\alpha \in \mathbb{R}$ s.t. $f(\alpha) = 0$, in a computational way. Most common approaches are *iterative*, since there is no explicit solving formula for $p \in \mathbb{R}^n$ with $n \geq 5$ for Abel's theorem.



Bisection method (Linear convergence)

This method is used to compute the root of a *continuous* function f on $[a, b]$, i.e., the point α such that $f(\alpha) = 0$. We assume that $f : [a, b] \to \mathbb{R}$ and $a < b$. If $f(a)f(b) < 0$, since f is continuous, we know that there exists (at least) one root α of f in the interval $[a, b]$, thanks to the following

Property (Theorem of zeros for continuous functions)**.** *Given a continuous function* $f : [a, b] \to \mathbb{R}$*, such that* $f(a)f(b) < 0$*, then* $\exists \alpha \in (a, b)$ *such that* $f(\alpha) = 0$*.*



Starting from $I^{(0)} = [a, b]$, the **bisection method** generates a sequence of subintervals $I^{(k)} = [a^{(k)}, b^{(k)}]$, $k \geq 0$, with $I^{(k)} \subset I^{(k-1)}$, $k \geq 1$, and enjoys the property that $f(a^{(k)})f(b^{(k)}) < 0$. Precisely,

1. set $a^{(0)} = a$, $b^{(0)} = b$ and $x^{(0)} = \frac{a^{(0)}+b^{(0)}}{2}$,
2. then, for $k \geq 0$, if $f(x^{(k)}) = 0$, then $x^{(k)}$ is the zero.
3. if $f(x^{(k)}) \neq 0$, then:
   a. if $f(x^{(k)})f(b^{(k)}) < 0 \Leftrightarrow f(a^{(k)})f(x^{(k)}) > 0 \Rightarrow$ the zero $\alpha \in (x^{(k)}, b^{(k)})$ and we define $a^{(k+1)} = x^{(k)}, b^{(k+1)} = b^{(k)}$,
   b. if $f(a^{(k)})f(x^{(k)}) < 0 \Leftrightarrow f(x^{(k)})f(b^{(k)}) > 0 \Rightarrow$ the zero $\alpha \in (a^{(k)}, x^{(k)})$ and we define $a^{(k+1)} = a^{(k)}, b^{(k+1)} = x^{(k)}$,
   c. finally, set $x^{(k+1)} = (a^{(k+1)} + b^{(k+1)})/2$.

We generate a sequence of intervals whose length is halved at each step, with $x^{(k)}$ being the midpoint at step k. By the divisions of this type, we construct the sequence $x^{(0)}, x^{(1)}, \dots, x^{(k)}$ such that $\lim_{k\to\infty} x^{(k)} = \alpha$ and that satisfies, for all k,

$$\boxed{|e^{(k)}| = |x^{(k)} - \alpha| \leq \frac{1}{2} I^{(k)} = \frac{b^{(k)} - a^{(k)}}{2} = \frac{b-a}{2^{k+1}}},$$

which is the *absolute error*, th error of estimation, at step k. This implies that $\lim_{k\to\infty} |e^{(k)}| = 0$, so the bisection method is therefore **globally convergent**.

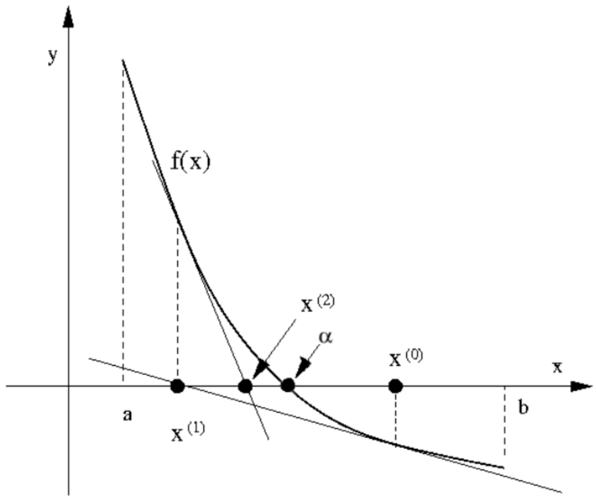
In order to ensure that the error is $|e^{(k)}| < \varepsilon$, we carry out k_{min} iterations at least:

$$k_{\text{min}} > \log_2\left(\frac{b-a}{\varepsilon}\right) - 1$$

The error doesn't decrease monotonically. The only possible stopping criterion is controlling the size of $I^{(k)}$.

Newton’s method (Quadratic or linear convergence)

It is used to compute the root of a function f by using the values of f and f', and thus it is more efficient than the bisection method.



Let $f : \mathbb{R} \to \mathbb{R}$ be a differentiable function. Let $x^{(0)}$ be an initial guess, which is sufficiently close to α given f (estimated maybe through the graph or the bisection method). Let us consider the equation $y(x)$ which passes through the point $(x^{(k)}, f(x^{(k)}))$ and which has slope $f'(x^{(k)})$ (*linearized* version of problem):

$$y(x) = f'(x^{(k)})(x - x^{(k)}) + f(x^{(k)}).$$

We define $x^{(k+1)}$ by the point where this line intersects the axis x, i.e. $y(x^{(k+1)}) = 0$, since we are trying to approximate the root of the function. We deduce that:

$$\boxed{x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}}, \qquad k = 0, 1, 2, \dots$$

Starting from the point $x^{(0)}$, the sequence $\{x^{(k)}\}$ converges the the root of f. This method is called **Newton - Rapson method**. Actually, the convergence of this method depends on the *property of the function* and on the *initial guess*.

Secant method (Super-linear convergence)

Let f be a *continuous* function with root α with $m = 1$ (for super-linearity) and $f'(x) \neq 0 \; \forall x \in I(\alpha)$, and let's select the initial point $x^{(0)}$ in a suitable $I(\alpha)$. In case $f'(x)$ is not available we can replace its value with an incremental ratio based on previous values:

$$\boxed{x^{(k+1)} = x^{(k)} - \left(\frac{f(x^{(k)}) - f(x^{(k-1)})}{x^{(k)} - x^{(k-1)}} \right)^{-1} f(x^{(k)})}, \quad k = 0, 1, 2, \dots$$

If $m = 1$ and $f \in C^2(I(\alpha))$, $\exists c > 0$ s.t. $|x^{(k+1)} - \alpha| \leq c|x^{(t)} - \alpha|^p$, with $p \approx 1.618$.

Otherwise, the method converges linearly.

Systems of nonlinear equations

Given $f_1, \dots, f_n$ nonlinear functions in $x_1, \dots, x_n$, we can set $\bar{f} = (f_1, \dots, f_n)^T$ and $\bar{x} = (x_1, \dots, x_n)^T$ to write a system as

$$\bar{f}(\bar{x}) = 0.$$

We can extend the Newton method to this system by replacing the derivative f' with the *Jacobian matrix* $J_{\bar{f}}$, as $(J_{\bar{f}})_{ij} = \frac{\partial f_i}{\partial x_j}$ for $i, j = 1, \dots, n$.

The secant method can also be adopted by recursively defining matrices B_k which are suitable approximations of $J_{\bar{f}}(x^{(0)})$ (**Broyden method**). This belongs to the family of **Quasi-Newton methods**.

Fixed point iterations

A general method for finding the roots of a nonlinear equation $f(x) = 0$ is the transformation in an equivalent problem $x - \phi(x) = 0$, where the auxiliary function $\phi : [a, b] \to \mathbb{R}$ must have the following property:

$$\phi(\alpha) = \alpha \quad \text{if and only if} \quad f(\alpha) = 0.$$

The point α is called a **fixed point** of ϕ, while ϕ is called the **iteration function**. Searching the zeros of f is reduced to the problem of determining the fixed points of ϕ.

It could be computed by the following algorithm:

$$\boxed{x^{(k+1)} = \phi(x^{(k)})}, \quad k \geq 0.$$

Indeed, if $x^{(k)} \to \alpha$ and if ϕ is *continuous* on $[a, b]$, then the limit α satisfies $\phi(\alpha) = \alpha$. So, starting from the point $x^{(0)}$, the sequence $\{x^{(k)}\}$ converges to the fixed point α.

The Newton method is a fixed point method: $x^{(k+1)} = \phi(x^{(k)})$ for the function

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

Let α be a zero of f, i.e. such that $f(\alpha) = 0$. Note that $\phi'(\alpha) = 0$, when $f'(\alpha) \neq 0$. Indeed,

$$\phi'(x) = 1 - \frac{[f'(x)]^2 - f(x)f''(x)}{[f'(x)]^2} = 1 - 1 + \frac{f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2}.$$

Proposition 1 (Global convergence).

1. *Assume that $\phi(x)$ is continuous on $[a, b]$ and such that $\phi(x) \in [a, b]$ for all $x \in [a, b]$; then there exists at least one fixed point $\alpha \in [a, b]$ of ϕ.*
2. *If ϕ is Lipschitz continue with constant $L < 1$ (**asymptotic convergence factor**), that is, if $\exists L < 1$ such that*

$$|\phi(x_1) - \phi(x_2)| \leq L|x_1 - x_2| \; \forall x_1, x_2 \in [a, b],$$

then there exists a unique fixed point $\alpha \in [a, b]$ and the sequence $x^{(k+1)} = \phi(x^{(k)}), k \geq 0$ converges to α, for any initial guess $x^{(0)} \in [a, b]$.

Proof.

1. The function $g(x) = \phi(x) - x$ is continuous in $[a, b]$ and, thanks to the assumption made on the range of ϕ, it holds $g(a) = \phi(a) - a \geq 0$ and $g(b) = \phi(b) - b \leq 0$. By applying the theorem of zeros of continuous functions, we can conclude that g has at least one zero in $[a, b]$, i.e. $\exists \alpha \in [a, b]$ such that

$$0 = g(\alpha) = \phi(\alpha) - \alpha \quad \iff \quad \phi(\alpha) = \alpha$$

so ϕ has at least one fixed point in $[a, b]$.

2. Indeed, should two different fixed points α_1 and α_2 exist, then

$$|\alpha_1 - \alpha_2| = |\phi(\alpha_1) - \phi(\alpha_2)| \leq L|\alpha_1 - \alpha_2| < |\alpha_1 - \alpha_2|$$

(since, in order, α_i is a fixed point of ϕ, ϕ is Lipschitz continuous and $L < 1$) which cannot be. So there exists a unique fixed point $\alpha \in [a, b]$ of ϕ.

Let $x^{(0)} \in [a, b]$ and $x^{(k+1)} = \phi(x^{(k)})$. We have

$$0 \leq |x^{(k+1)} - \alpha| = |\phi(x^{(k)}) - \phi(\alpha)| \leq L|x^{(k)} - \alpha| \leq \ldots \leq L^{k+1}|x^{(0)} - \alpha|,$$

i.e. $\forall k \geq 0$:

$$\frac{|x^{(k)} - \alpha|}{|x^{(0)} - \alpha|} \leq L^k.$$

For the convergence analysis and because $L < 1$, for $k \to \infty$, we obtain

$$\lim_{k \to \infty} |x^{(k)} - \alpha| \leq \lim_{k \to \infty} L^k |x^{(0)} - \alpha| = 0.$$

So, $\forall x^{(0)} \in [a, b]$, the sequence $\{x^{(k)}\}$ defined by $x^{(k+1)} = \phi(x^{(k)}), k \geq 0$ converges to α when $k \to \infty$.

□

The Proposition 1 ensures the convergence of the sequence $\{x^{(k)}\}$ at the root α for *any* choice of the initial guess $x^{(0)} \in [a, b]$. So it is a result of **global convergence**.

Remark. *If $\phi(x)$ is differentiable in $[a, b]$ and $\exists K < 1$ such that $|\phi'(x)| \leq K \; \forall x \in [a, b]$, then the condition (2) of the Proposition 1 is satisfied. This assumption is stronger, but is more often used in practice because it is easier to check.*

Definition. For a sequence of real numbers $\{x^{(k)}\}$ that converges, $x^{(k)} \to \alpha$, we say that **the convergence to α is linear** if exists a constant $C < 1$ such that, for k that is large enough

$$\boxed{|x^{(k+1)} - \alpha| \leq C|x^{(k)} - \alpha|}.$$

If exists a constant $C > 0$ such that the inequality

$$\boxed{|x^{(k+1)} - \alpha| \leq C|x^{(k)} - \alpha|^2}$$

is satisfied, we say that **the convergence is quadratic**.
In general, **the convergence is with order p**, with $p \geq 1$, if exists a constant $C > 0$ (with $C < 1$ when $p = 1$) such that the following inequality is satisfied

$$|x^{(k+1)} - \alpha| \leq C|x^{(k)} - \alpha|^p.$$

Proposition 2 (Ostrowski's theorem: local convergence). *Let ϕ be a continuous and differentiable function on $[a, b]$ and α be a fixed point of ϕ. If $|\phi'(\alpha)| < 1$, then there exists $\delta > 0$ such that, for all $x^{(0)}$, $|x^{(0)} - \alpha| \leq \delta$, the sequence $\{x^{(k)}\}$ defined by $x^{(k+1)} = \phi(x^{(k)})$ converges to α when $k \to \infty$. Moreover, it holds*

$$\boxed{\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{x^{(k)} - \alpha} = \phi'(\alpha)}. \tag{1}$$

Proof. The first parts follow directly from the previous theorem, the Proposition 1. Let's prove the property (1). For the Taylor series expansion (or for the Lagrange theorem), for any $k \geq 0$ there exists a value $\eta^{(k)}$ between α and $x^{(k)}$ such that

$$x^{(k+1)} - \alpha = \phi(x^{(k)}) - \phi(\alpha) = \phi(\eta^{(k)})(x^{(k)} - \alpha).$$

Since $\eta^{(k)}$ is included between α and $x^{(k)}$, we have that $\lim_{k\to\infty} \eta^{(k)} = \alpha$, and remembering that ϕ' in continuous in a neighbourhood of α, this implies that

$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{x^{(k)} - \alpha} = \lim_{k\to\infty} \phi'(\eta^{(k)}) = \phi'(\alpha),$$

that is (1).

$\square$

Note that, if $0 < |\phi'(\alpha)| < 1$, then for any constant C such that $|\phi'(\alpha)| < C < 1$, if k is large enough, we have:

$$|x^{(k+1)} - \alpha| \leq C|x^{(k)} - \alpha|.$$

This is a way to compute C locally.

Proposition 3 (Quadratic convergence). *Let ϕ be a twice differentiable function on $[a, b]$, so $\phi \in C^2([a, b])$, and α be a fixed point of ϕ. Let us consider that $x^{(0)}$ converges locally. If $\phi'(\alpha) = 0$ and $\phi''(\alpha) \neq 0$, then the fixed point iterations converges with order 2 and*

$$\boxed{\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \frac{\phi''(\alpha)}{2}}.$$

Proof. Using the Taylor series for ϕ with $x = \alpha$, we have

$$x^{(k+1)} - \alpha = \phi(x^{(k)}) - \phi(\alpha) = \phi'(\alpha)(x^{(k)} - \alpha) + \frac{\phi''(\eta^{(k)})}{2}(x^{(k)} - \alpha)^2$$

where $\eta^{(k)}$ is between $x^{(k)}$ and α. So, since $\phi'(\alpha) = 0$ and $\lim_{k\to\infty} \eta^{(k)} = \alpha$, we have

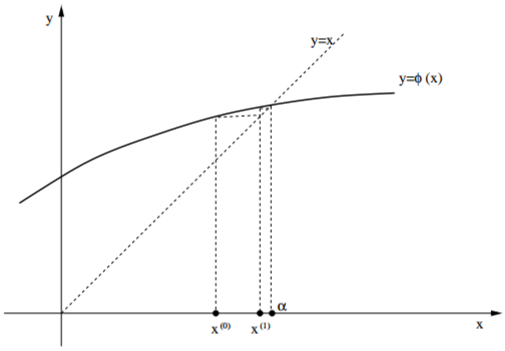
$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \lim_{k\to\infty} \frac{\phi''(\eta^{(k)})}{2} = \frac{\phi''(\alpha)}{2}.$$

$\square$

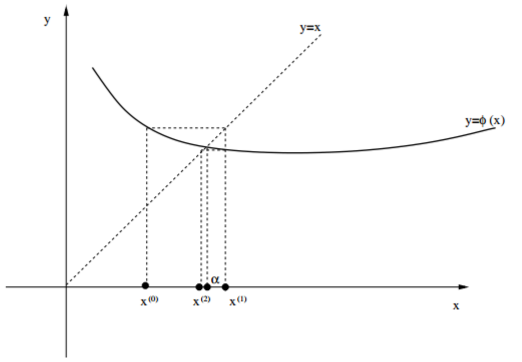
The value $|\phi'(\alpha)|$ influences the convergence: if $|\phi'(\alpha)| < 1$ we have that the method diverges. If $|\phi'(\alpha)| > 1$ then for (1) we have that $|x^{(k+1)} - \alpha| > |x^{(k)} - \alpha|$, thus no convergence is possible. While if $|\phi'(\alpha)| = 1$ no general conclusion can be stated since both convergence and non-convergence may be possible, depending on the problem at hand.

Convergent cases:

$$0 < \phi'(\alpha) < 1,$$

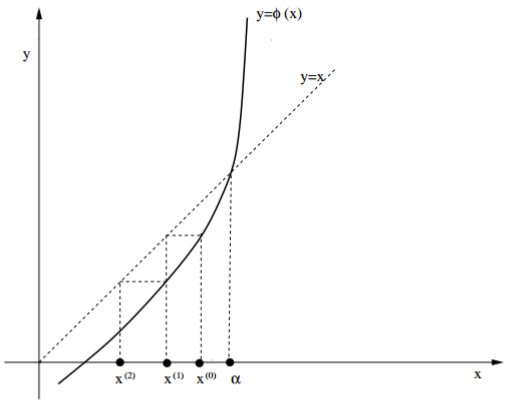


$$-1 < \phi'(\alpha) < 0.$$

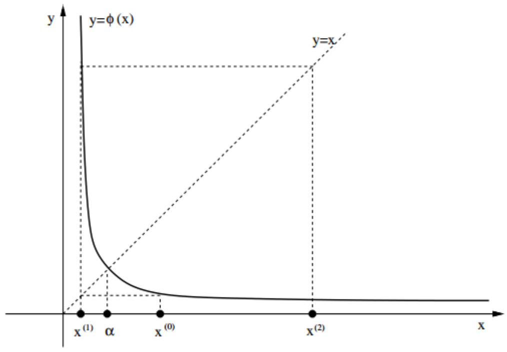


Divergent cases:

$$\phi'(\alpha) > 1,$$



$$\phi'(\alpha) < -1.$$



More about the Newton method

Theorem 1. *If f is twice differentiable ($f \in C^2([a,b])$), $f(\alpha) = 0$ and $f'(\alpha) \neq 0$, then there exists $\delta > 0$ such that, if $|x^{(0)} - \alpha| \leq \delta$, the sequence defined by the Newton method converges to α. Moreover, the convergence is quadratic; more precisely*

$$\boxed{\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \frac{f''(\alpha)}{2f'(\alpha)}}.$$

Proof. The property of convergence comes from the Proposition 2, while the quadratic convergence is a consequence of the Proposition 3, because $\phi'(\alpha) = 0$ and $\frac{\phi''(\alpha)}{2} = \frac{f''(\alpha)}{2f'(\alpha)}$.

□

Definition. Let α be a zero of f. Then α is said to have **multiplicity** m, with $m \in \mathbb{N}$, if

$$f(\alpha) = f'(\alpha) = \ldots = f^{(m-1)}(\alpha) = 0 \text{ and } f^{(m)}(\alpha) \neq 0.$$

A zero that has multiplicity $m = 1$ is called **simple zero**.

Remark. If the root α has multiplicity $m > 1$, that means $f'(\alpha) = 0$, the convergence of the Newton method is linear, not quadratic. To restore the quadratic convergence we can use the **modified Newton method**:

$$\boxed{x^{(k+1)} = x^{(k)} - m\frac{f(x^{(k)})}{f'(x^{(k)})}}, \quad k = 0, 1, 2, \ldots$$

where m is the multiplicity of α.

If the multiplicity m of α is unknown, there are other methods, the **adaptive Newton methods**, which can recover the quadratic order of convergence.

Stopping criteria

Suppose that $\{x^{(k)}\}$ is a sequence converging to a zero α of the function f. We provide some stopping criteria for terminating the iterative process that approximates α. In general, for all discussed methods, we can use two different stopping criteria: the iterations is completed when

$$|x^{(k+1)} - x^{(k)}| < \varepsilon \quad \textbf{(control of the increment)},$$

or

$$|f(x^{(k)})| < \varepsilon \quad \textbf{(control of the residual)},$$

where ε is a fixed tolerance.

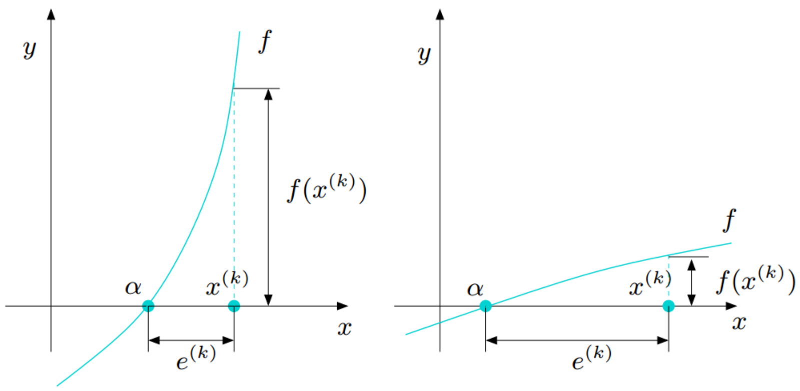
Below, ε is a fixed tolerance on the approximate calculation of α and $e^{(k)} = \alpha - x^{(k)}$ denotes the **absolute error** of the iteration k. We shall moreover assume that f is continuously differentiable in a suitable neighborhood of the root.

Control of the residual: *the iterative process terminates at the first step k such that $|f(x^{(k)})| < \varepsilon$.*

In the case of simple roots, the error is bound to the residual by the factor $1/|f'(\alpha)|$ so that the following conclusions can be drawn:

1. if $|f'(\alpha)| \simeq 1$, then $|e^{(k)}| \simeq \varepsilon$; therefore, the test provides a satisfactory indication of the error;
2. if $|f'(\alpha)| \ll 1$, the test is not reliable since $|e^{(k)}|$ could be quite large with respect to ε (the test is too weak);
3. if, finally, $|f'(\alpha)| \gg 1$, we get $|e^{(k)}| \ll \varepsilon$ and the test is too restrictive (the test is too strong).

Two cases where the residual is a bad estimator of the error: $|f'(x)| \gg 1$ (left), and $|f'(x)| \ll 1$ (right)) with x near to α:



Control of the increment: *the iterative process terminates as soon as $|x^{(k+1)} - x^{(k)}| < \varepsilon$.*

Using fixed point iterations, where $x^{(k+1)} = \phi(x^{(k)})$, we obtain the following estimation of the absolute error $e^{(k)}$ using the mean value theorem:

$$e^{(k+1)} = \alpha - x^{(k+1)} = \phi(\alpha) - \phi(x^{(k)}) = \phi'(\xi^{(k)})(\alpha - x^{(k)}) = \phi'(\xi^{(k)})e^{(k)},$$

where $\xi^{(k)}$ lies between $x^{(k)}$ and α. Then,

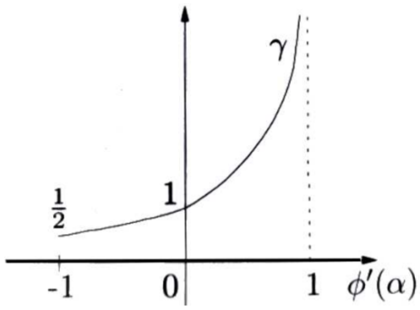
$$x^{(k+1)} - x^{(k)} = x^{(k+1)} - \alpha + \alpha - x^{(k)} = e^{(k)} - e^{(k+1)} = \left(1 - \phi'(\xi^{(k)})\right) e^{(k)}$$

so that, assuming that if k is large enough, we have $\phi'(\xi^{(k)}) \approx \phi'(\alpha)$, so it follows that

$$e^{(k)} \approx \frac{1}{(1-\phi'(\alpha))}(x^{(k+1)} - x^{(k)}).$$

We can plot the graph of $\frac{1}{(1-\phi'(\alpha))}$ and comment on the relevance of the stopping criteria based on the increment:

- if $\phi'(\alpha)$ is close to 1 the test is unsatisfactory
- for methods of order 2, for which $\phi'(\alpha) = 0$, the criteria is optimal: it provides an optimal balancing between increment and error. This is the case of the Newton method, for which if α is a simple zero, we have the estimation
$$|x^{(k+1)} - x^{(k)}| \approx |(1-\phi'(\alpha))e^{(k)}| = |e^{(k)}|.$$
- if $-1 < \phi'(\alpha) < 0$ the criteria is still satisfactory.



Aitken's method

Consider a fixed-point iteration that is linearly converging to a zero α of a given function f. Denote by λ an approximation of $\phi'(\alpha)$ to be suitably determined.

If ϕ converges linearly to α, since for Proposition 2 it holds $\lim_{k\to\infty} \frac{x^{(k+1)}-\alpha}{x^{(k)}-\alpha} = \phi'(\alpha)$, there must be a λ s.t.

$$\phi(x^{(k)}) - \alpha = x^{(k+1)} - \alpha = \phi'(\alpha)(x^{(k)} - \alpha) \simeq \lambda(x^{(k)} - \alpha), \quad \text{for } k \geq 1.$$

This allows us to obtain a better estimate of $x^{(k+1)}$ than $\phi(x^{(k)})$. Thus

$$\alpha \simeq x^{(k)} + \frac{\phi(x^{(k)}) - x^{(k)}}{1-\lambda}$$

Let us consider, for $k \geq 2$, the following ratio

$$\lambda^{(k)} = \frac{\phi(\phi(x^{(k)})) - \phi(x^{(k)})}{\phi(x^{(k)}) - x^{(k)}},$$

and check that (see book)

$$\lim_{k\to\infty} \lambda^{(k)} = \phi'(\alpha).$$

We have that

$$x^{(k+1)} = x^{(k)} - \frac{(\phi(x^{(k)}) - x^{(k)})^2}{\phi(\phi(x^{(k)})) - 2\phi(x^{(k)}) + x^{(k)}}, \quad k \geq 0$$

that is the **Aitken’s extrapolation formula** or the **Steffenson's method**.

The derived function $\phi_\Delta(x)$ has the same α as $\phi(x)$, but converges faster:

- *linear* $\phi \longrightarrow$ *quadratic* ϕ_Δ
- $p \geq 2 \longrightarrow 2p - 1 \ \phi_\Delta$
- *linearly* with $m \geq 2 \ \phi \longrightarrow$ *linearly* with $L = 1 - 1/m \ \phi_\Delta$

It may converge even if normal fixed-point iteration diverges.

The rope method

This method is obtained by replacing $f'(x^{(k)})$ by a fixed q in the Newton method:

$$x^{(k+1)} = x^{(k)} - \frac{1}{q} f(x^{(k)}), \quad k = 0, 1, 2, \ldots$$

We can take, for example, $q = f'(x^{(0)})$ or $q = \frac{f(b)-f(a)}{b-a}$, in the case when we search a zero in the interval $[a, b]$.

Remark. The rope method is also a fixed point method for

$$\phi(x) = x - \frac{1}{q} f(x).$$

So, we have $\phi'(x) = 1 - \frac{1}{q} f'(x)$ and thanks to the Proposition 2, we obtain that the method converges if the following condition is satisfied:

$$|\phi'(\alpha)| = \left|1 - \frac{1}{q} f'(\alpha)\right| < 1.$$