Nonlinear equations

Numerical Analysis

Profs. Gianluigi Rozza - Luca Heltai

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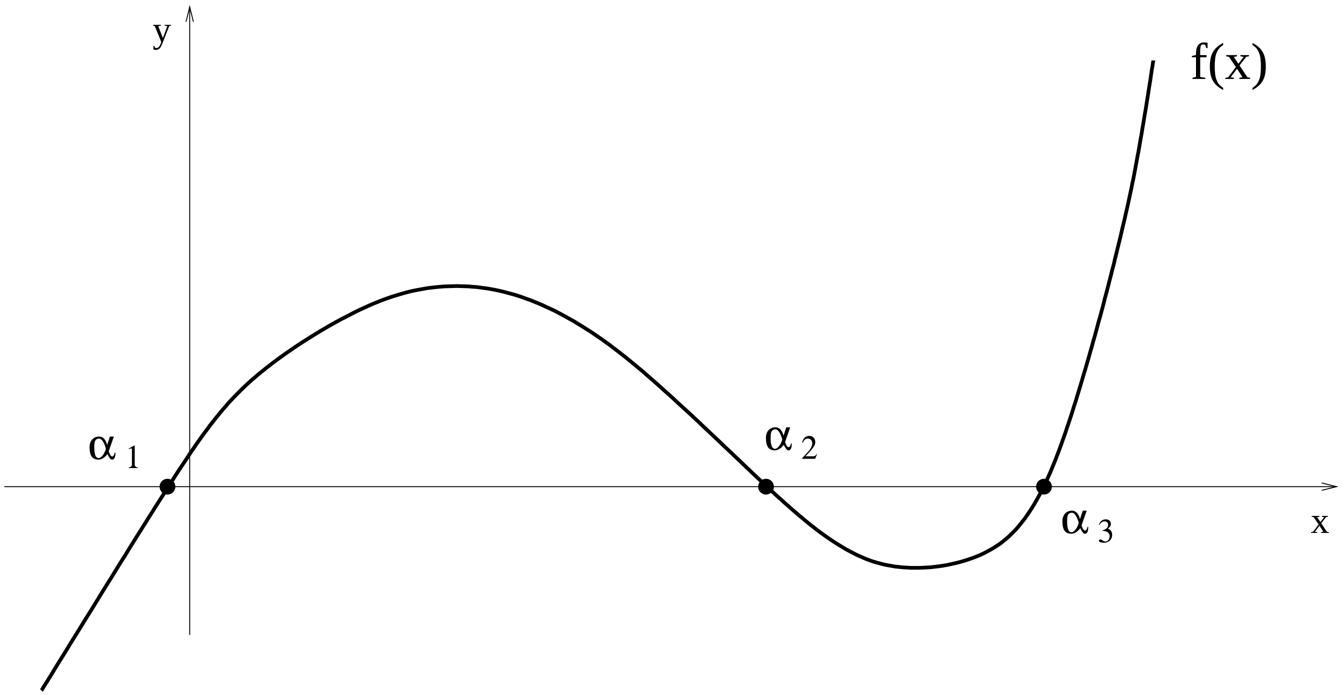
Nonlinear equations

Objective: Find the root of scalar (or vector) non-linear functions, i.e., find $\alpha \in \mathbb{R}$ such that $f(\alpha) = 0$.



Examples and motivation

Example 1 (Interest rates)**.** We want to compute the mean interest rate I of a portfolio over several years. We invest $v = 1000$ Euro every year. After 5 years we end up with $M = 6000$ Euro.
The relation between M, v, I and the number of years n is

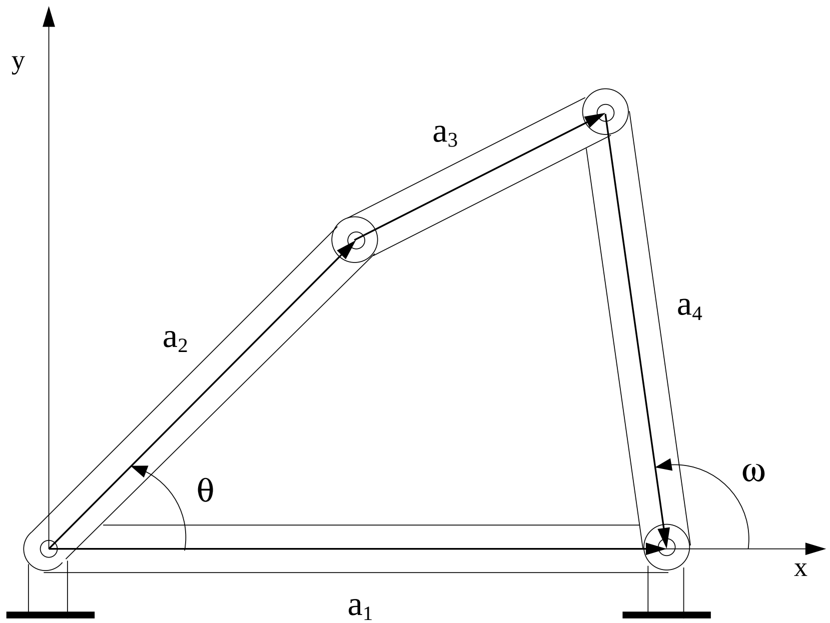
$$M = v\sum_{k=1}^{n}(1+I)^k = v\frac{1+I}{I}\left[(1+I)^n - 1\right]$$

This can be rewritten as: *find I such that*

$$f(I) = M - v\frac{1+I}{I}\left[(1+I)^n - 1\right] = 0 \qquad (1)$$

Therefore we have to solve a nonlinear equation in I, for which we can't find an analytical solution.

Example 2 (Rods system). Let us consider the mechanical system represented by four rigid rods



For any admissible angle ω, we want to compute the angle θ between $\mathbf{a}_1$ and $\mathbf{a}_2$.
Thanks to the vector identity

$$\mathbf{a}_1 - \mathbf{a}_2 - \mathbf{a}_3 - \mathbf{a}_4 = 0$$

and keeping $\mathbf{a}_1$ on the x-axis, we can derive the following equation: involving ω and θ:

$$\frac{a_1}{a_2} cos(\omega) - \frac{a_1}{a_4} cos(\theta) - cos(\omega - \theta) = -\frac{a_1^2 + a_2^2 - a_3^2 + a_4^2}{2a_2 a_4} \tag{2}$$

where a_i is the length of the ith rod. Equation (2) is nonlinear and can be solved only for particular values of ω. For a general ω it is not possible to find an analytic solution.

Example 3 (State equation of a gas). We want to determine the volume V occupied by a gas at temperature T and pressure p. The state equation (i.e. the equation that relates p, V et T) is

$$\left[p + a\left(\frac{N}{V}\right)^2\right](V - Nb) = kNT \, ,$$

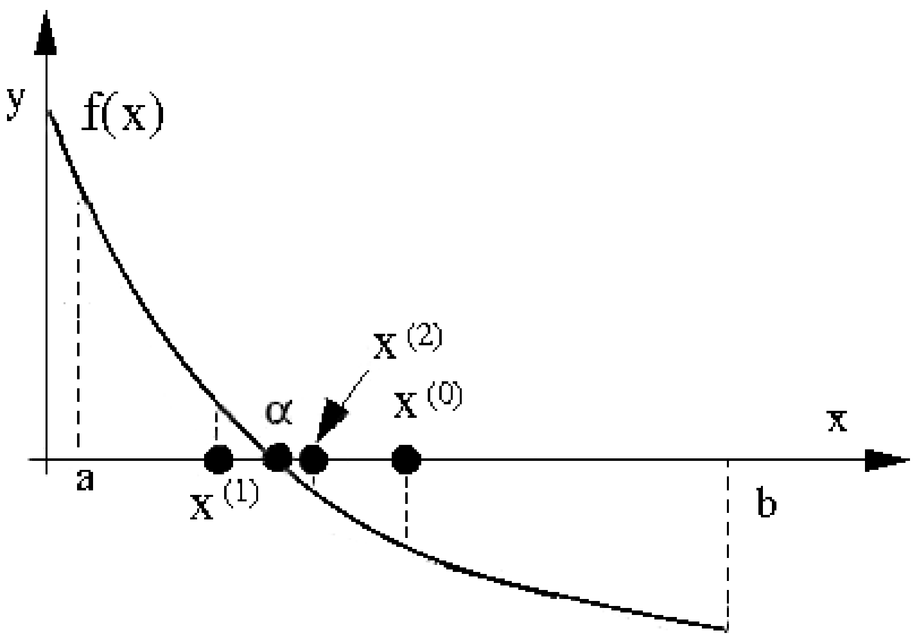
where a and b are two coefficients that depend on the specific gas, N is the number of molecules which are contained in the volume V and k is the Boltzmann constant. We need therefore to solve a non-linear equation whose root is V.

Bisection method

(Book Sec. 2.2)

This method is used to compute the root of a continuous function f, i.e., the point α such that $f(\alpha) = 0$. We can build a *sequence* $x^{(0)}, x^{(1)}, \ldots, x^{(k)}$, ($x^{(0)}$ such that $\lim_{k\to\infty} x^{(k)} = \alpha$.

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).



Then

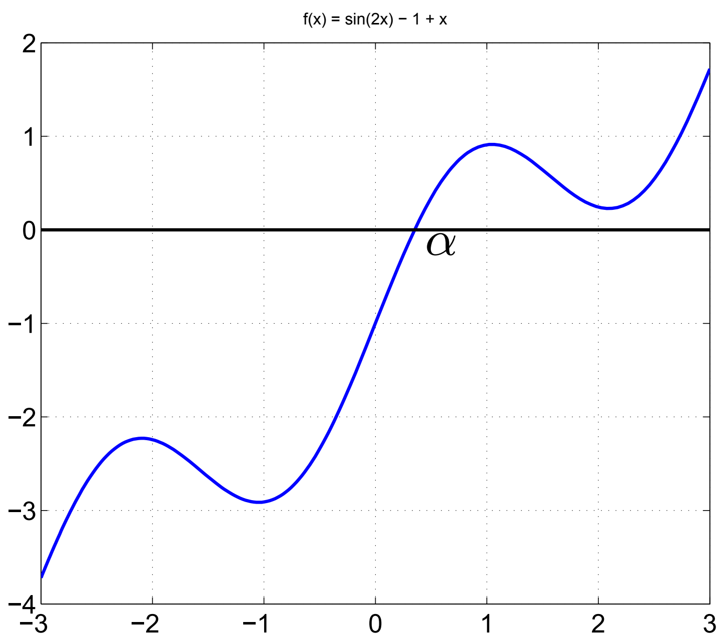
1. We set $a^{(0)} = a$, $b^{(0)} = b$ and $x^{(0)} = \frac{a^{(0)}+b^{(0)}}{2}$,
2. if $f(x^{(0)}) = 0$, then $x^{(0)}$ is the zero.
3. if $f(x^{(0)}) \neq 0$, then:
   (a) if $f(x^{(0)})f(a^{(0)}) > 0 \Rightarrow$ the zero $\alpha \in (x^{(0)}, b^0)$ and we define $a^{(1)} = x^{(0)}$, $b^{(1)} = b^{(0)}$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

By the divisions of this type, we construct the sequence $x^{(0)}, x^{(1)}, \dots, x^{(k)}$ that satisfies for all k,

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

Example 4. We want to find the zero of the function $f(x) = \sin(2x) - 1 + x$. We draw the graph of the function f using the following commands in Matlab/Octave:

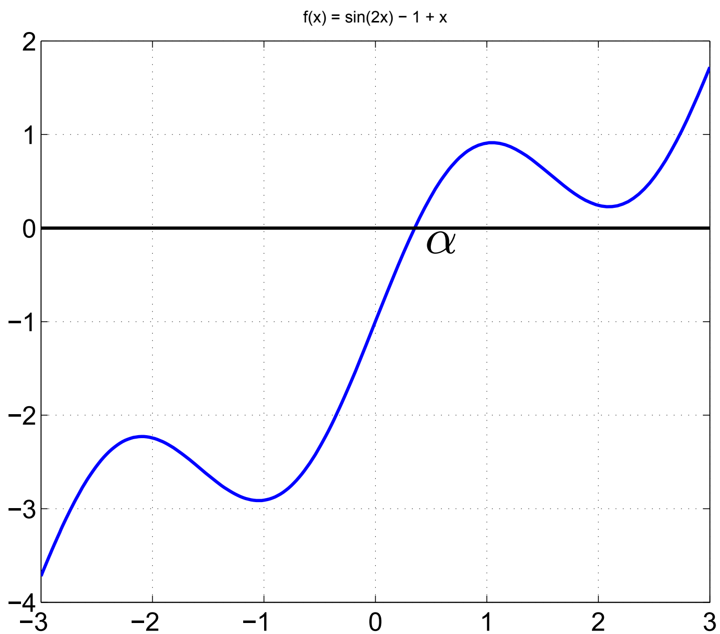
```
>> f = @(x) sin(2*x) -1 + x;
>> x=-3:0.1:3;
>> plot(x,f(x)); grid on;
```



If we appply the bisection method in the interval $[-1, 1]$ with a tolerance 10^{-8} and maximum number of iterations $k_{max} = 1000$

```
>> [zero,res,niter]=bisection(f,-1,1,1e-8,1000);
```

We find the value $\alpha = 0.352288462$ after 27 iterations.



Newton's method

(Chapt. 2.3 of the book)

Let $f : \mathbb{R} \to \mathbb{R}$ be a differentiable function.
Let $x^{(0)}$ be an initial guess. Let us consider the equation $y(x)$ which passes through the point $(x^{(k)}, f(x^{(k)}))$ and which has the slope $f'(x^{(k)})$:

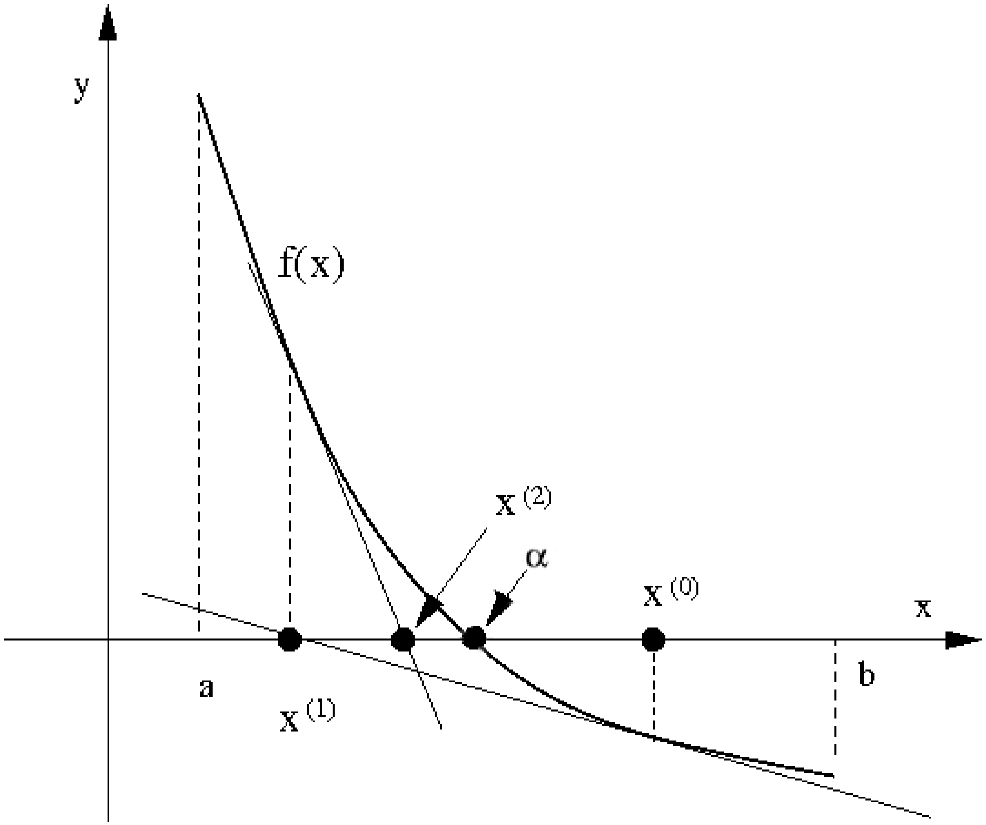
$$y(x) = f'(x^{(k)})(x - x^{(k)}) + f(x^{(k)}).$$

We define $x^{(k+1)}$ by the point where this line intersects the axis x, i.e. $y(x^{(k+1)}) = 0$. We deduce that:

$$\boxed{x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}, \quad k = 0, 1, 2 \ldots.} \tag{3}$$

Newton's method

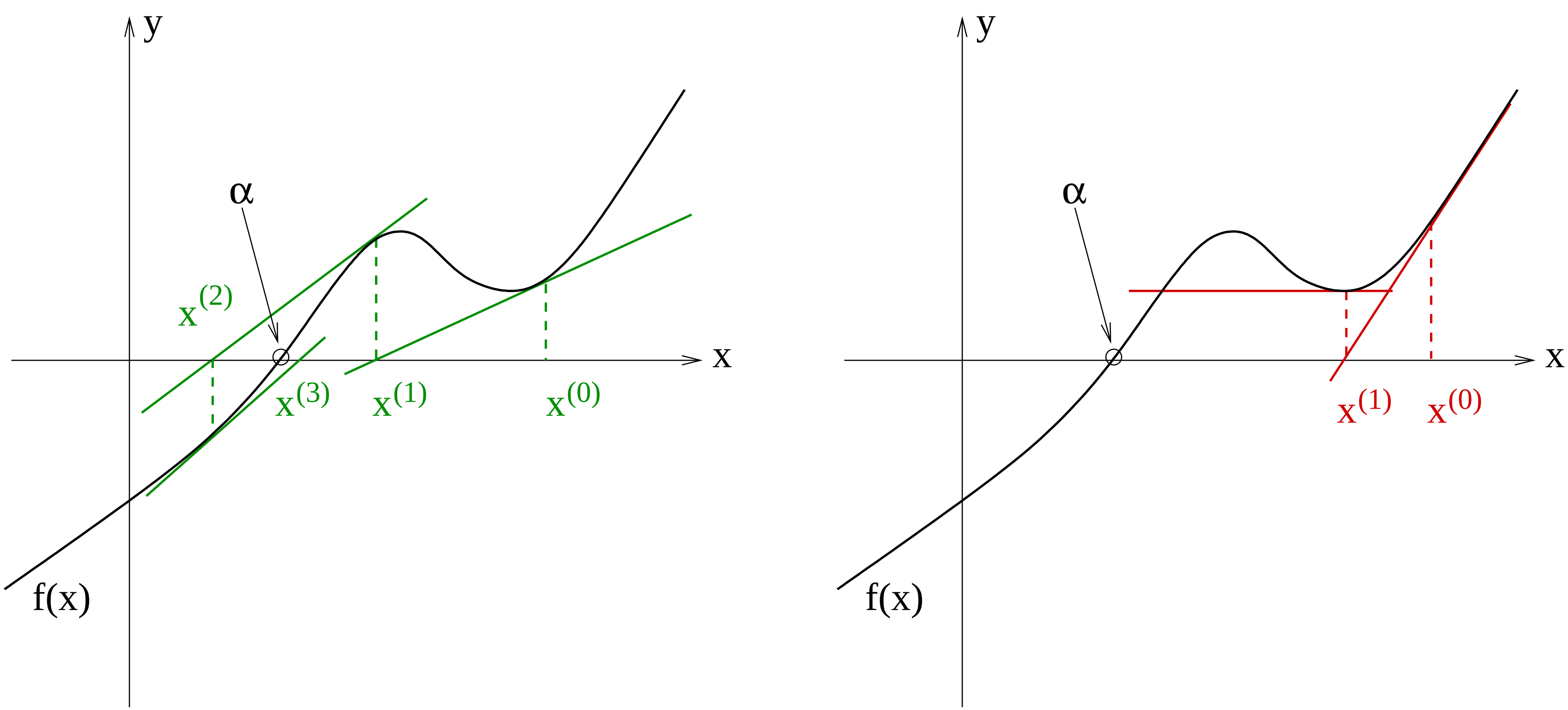
Starting from the point $x^{(0)}$, the sequence $\{x^{(k)}\}$ converges the the root of f



Convergence?

Does this method always converge?

- it depends on the property of the function;
- and on the initial guess.



Fixed point iterations.

(Chapt. 2.4 in the book)

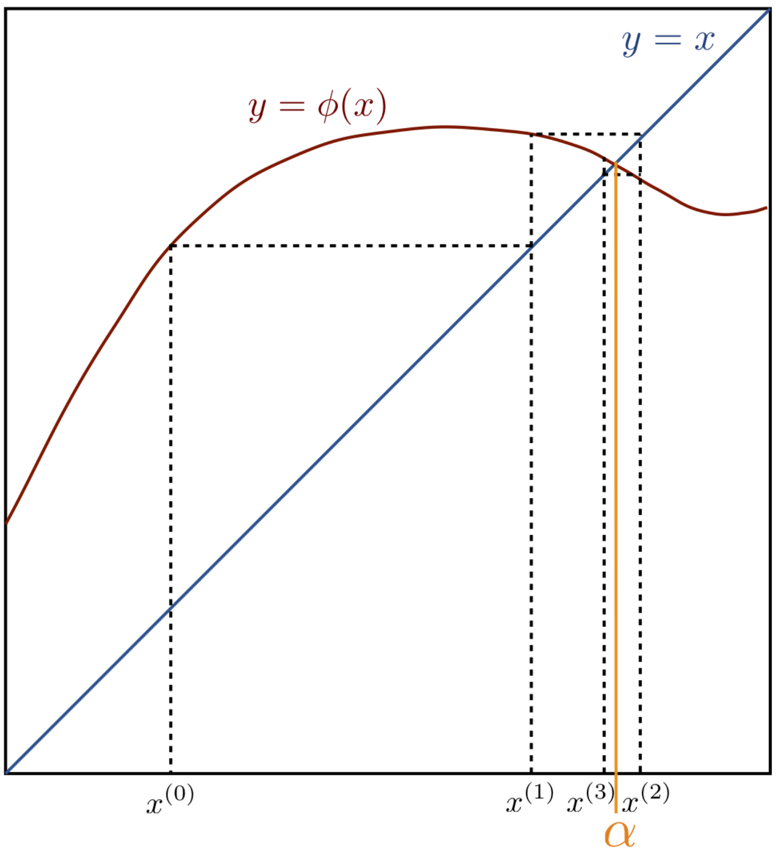
A general method for finding the roots of a nonlinear equation $f(x) = 0$ is the transformation an equivalent problem $x - \phi(x) = 0$, where the auxiliary function $\phi : [a, b] \to \mathbb{R}$ must have the following property :

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

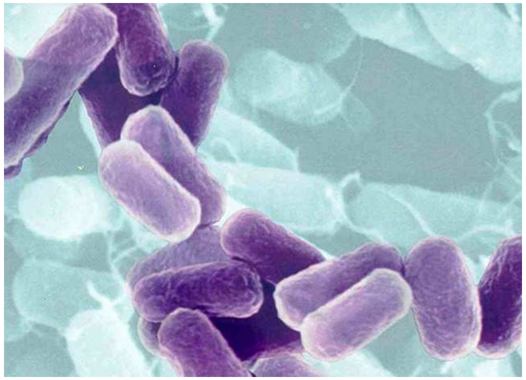
The point α is called *a fixed point* of ϕ. Searching the zeros of f is reduced to the problem of determining the fixed points of ϕ.

Idea : It could be computed by the following algorithm: $x^{(k+1)} = \phi(x^{(k)})$, $k \geq 0$. Indeed, if $x^{(k)} \to \alpha$ and if ϕ is continuous on $[a, b]$, then the limit α satisfies $\phi(\alpha) = \alpha$.

Starting from the point $x^{(0)}$, the sequence $\{x^{(k)}\}$ converges to the fixed point α



Example 5 (Population dynamics).



In the survey population (e.g. bacteria), we want to establish a link between the number of individuals in the generation x and the number of individuals in the next generation x^+:

$$x^+ = \phi(x) = xR(x), \tag{4}$$

where $R(x)$ represents the rate of growth (or decay) of the considered population.

Several models are available for $R(x)$:

- The Malthusian growth model (Thomas Malthus 1766-1834),

$$x^+ = \phi_1(x) = xR_1(x) \text{ with } R_1(x) = r, \quad r \text{ is a positive constant}$$

- the model of growth with limited resources (Pierre François Verhulst, 1804-1849),

$$x^+ = \phi_2(x) = xR_2(x) \text{ with } R_2(x) = r/(1 + x/K), \quad r > 0, K > 0$$

  that improve the Malthausian growth model by taking into account the growth of a population is limited by the resources.

- the predator/prey model

$$x^+ = \phi_3(x) = xR_3(x) \text{ with } R_3(x) = rx/(1 + (x/K)^2)$$

  that represents the change of the Verhulst model by presence of an antagonist population.

The dynamics of a population is defined by a iterative process, starting from a given initial guess ($x^{(0)}$),

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

where $x^{(k)}$ represents the number of individuals in k-th generation.
In addition, the steady states (equilibriums) x^* of a considered population are identified by the following problem,

$$x^* = \phi(x^*), \tag{5}$$

or equivalently,

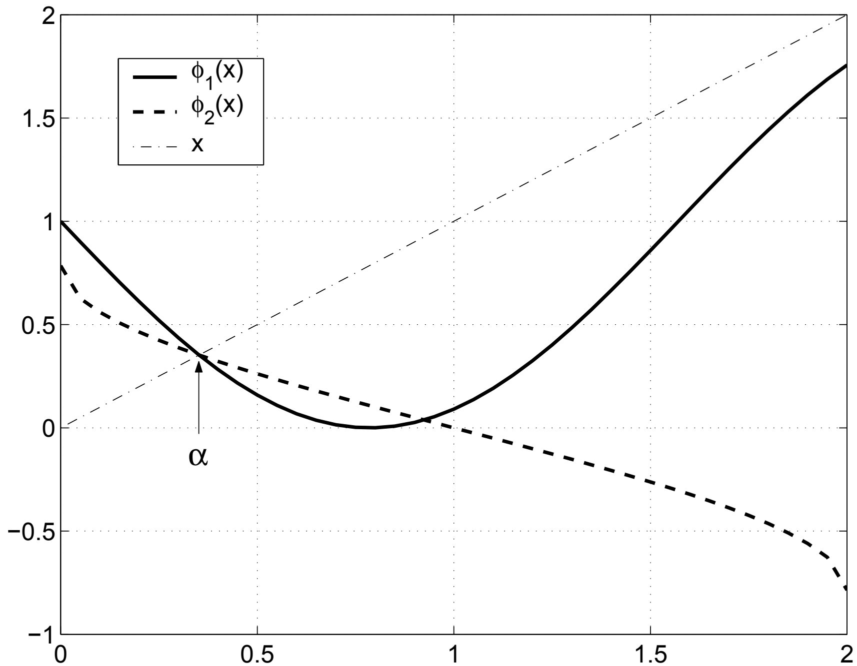
$$x^* = x^* R(x^*), \quad \text{i.e.} \quad R(x^*) = 1. \tag{6}$$

In both cases, we ask to solve a non-linear problem. In particular the problem is called the fixed point problem.

Example 6. We consider the equation $f(x) = \sin(2x) - 1 + x = 0$. We can rewrite it in two different fashions:

$$x = \phi_1(x) = 1 - \sin(2x)$$

$$x = \phi_2(x) = \frac{1}{2}\arcsin(1 - x), \qquad 0 \le x \le 1$$



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 $\exists L < 1$ 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 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. ϕ has at least one fixed point in $[a, b]$.

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

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

which cannot be. 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

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

i.e.

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

Because $L < 1$, for $k \to \infty$, we obtain

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

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 $k \to \infty$.

Remark 1.
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 condion 2 of the proposal (1) *is satisfied. This assumption is stronger, but is more often used in practice because it is easier to check.*

Definition 1. *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*

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

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

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

is satisfied, we say that convergence is quadratic.
In general, the convergence is with order p*,* $p \geq 1$*, 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. *(Local convergence - Theorem 2.1 in the book)*
Let ϕ be a continuous and differentiable function on $[a,b]$ and α be a fixed point of ϕ. If $\mid \phi'(\alpha) \mid < 1$, then there exists $\delta > 0$ such that, for all $x^{(0)}$, $\mid x^{(0)} - \alpha \mid \leq \delta$, the sequence $\{x^{(k)}\}$ defined by $x^{(k+1)} = \phi(x^{(k)})$ converges to α when $k \to \infty$.
Moreover, it holds

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

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

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

Proposition 3. *(Proposition 2.2 in the book)*
Let ϕ be a twice differentiable on $[a, b]$ 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 interations converges with order 2 and

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

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

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

where η is between $x^{(k)}$ and α. So, we have

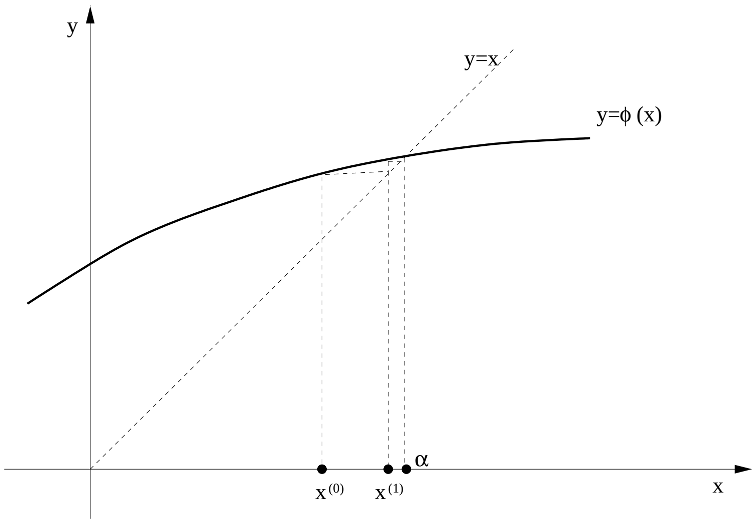
$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \lim_{k\to\infty} \frac{\phi''(\eta)}{2} = \frac{\phi''(\alpha)}{2}.$$

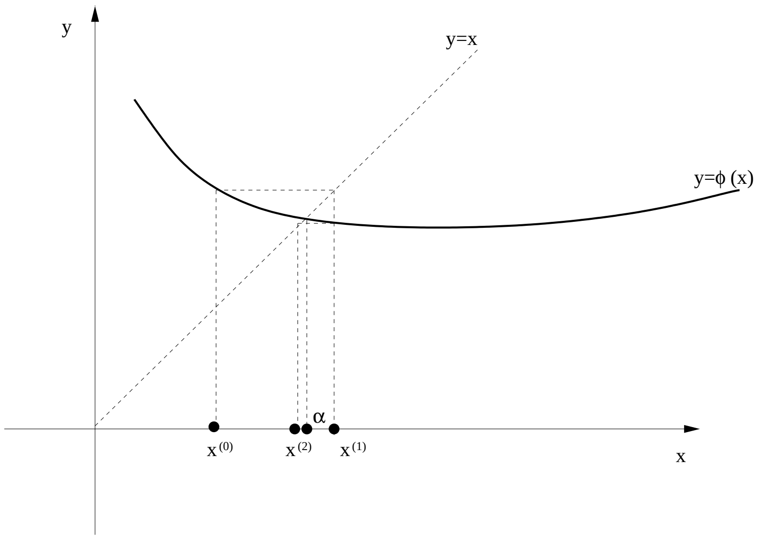
□

Some examples on how the value $|\ \phi'(\alpha)\ |$ influences the convergence

Convergent cases:

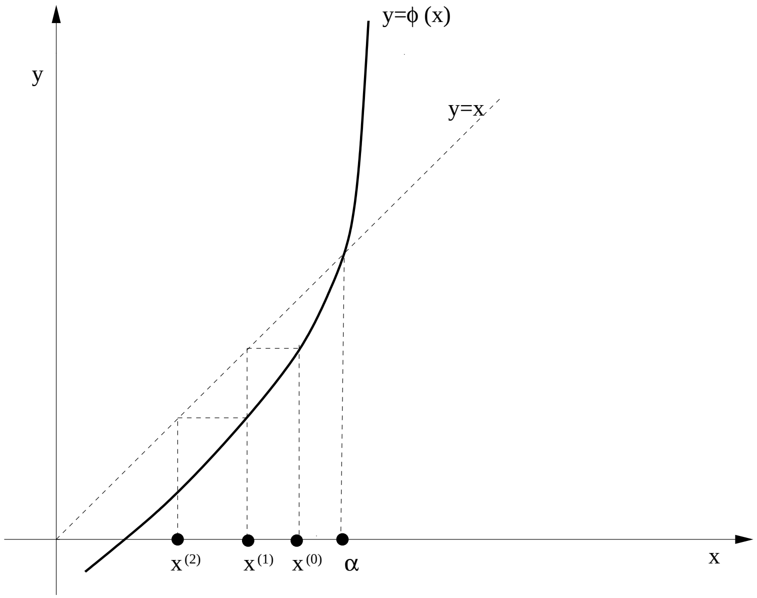
$$0 < \phi'(\alpha) < 1, \qquad -1 < \phi'(\alpha) < 0.$$

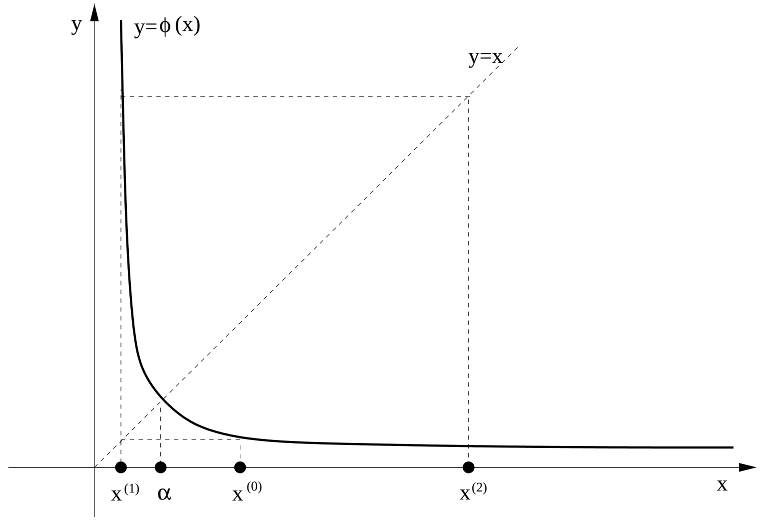




Divergent cases:

$$\phi'(\alpha) > 1, \qquad \phi'(\alpha) < -1.$$



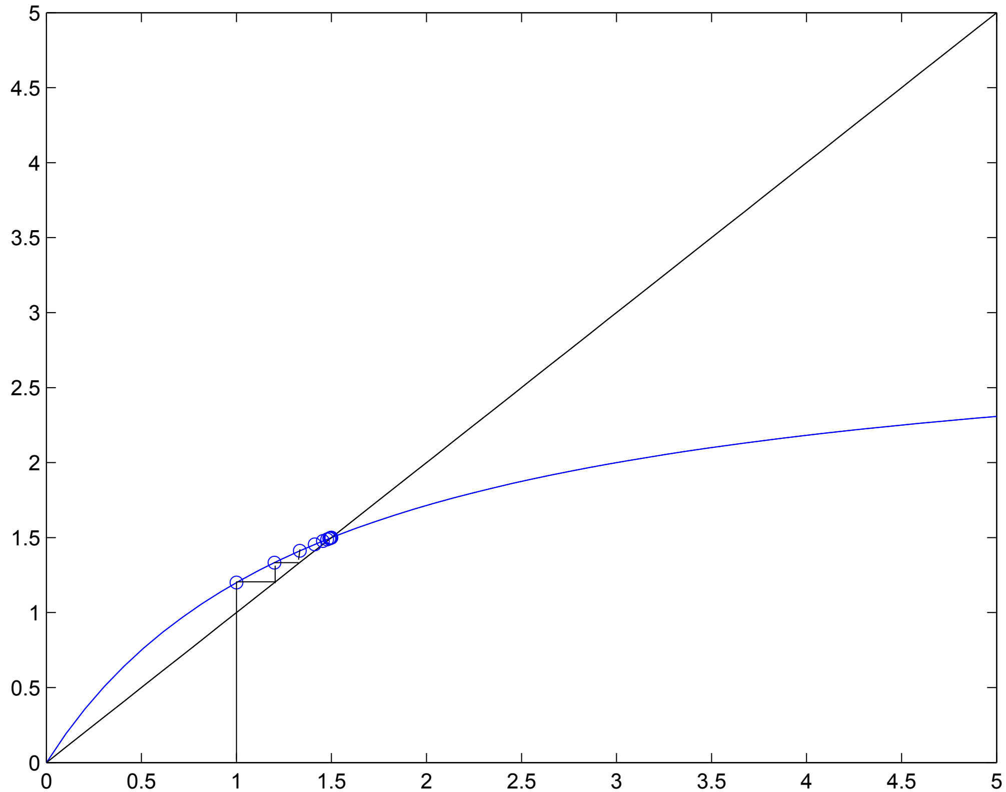


Example. 5 (suite) We apply the fixed point iterations on functions $\phi_2(x) = rx/(1 + x/K)$ and $\phi_3(x) = rx^2/(1 + (x/K)^2)$ that represent the Verhulst model and predator/prey model respectively, with $K = 1.5$ and $r = 2$. We consider the starting point $x^{(0)} = 1.0$.

```
>> phi2=@(x) x.*(2./(1+(x./1.5)));
>> phi3=@(x) x.*(2*x./(1+(x./1.5).^2));
>> x=linspace(0,5,50);
>> figure
>> plot(x,phi2(x),'b',x,x,'k');
>> [p2,res2,niter2]=fixpoint(phi2,1,1e-6,1000);
>> figure
>> plot(x,phi3(x),'b',x,x,'k');
>> [p3,res3,niter3]=fixpoint(phi3,1,1e-6,1000);
```

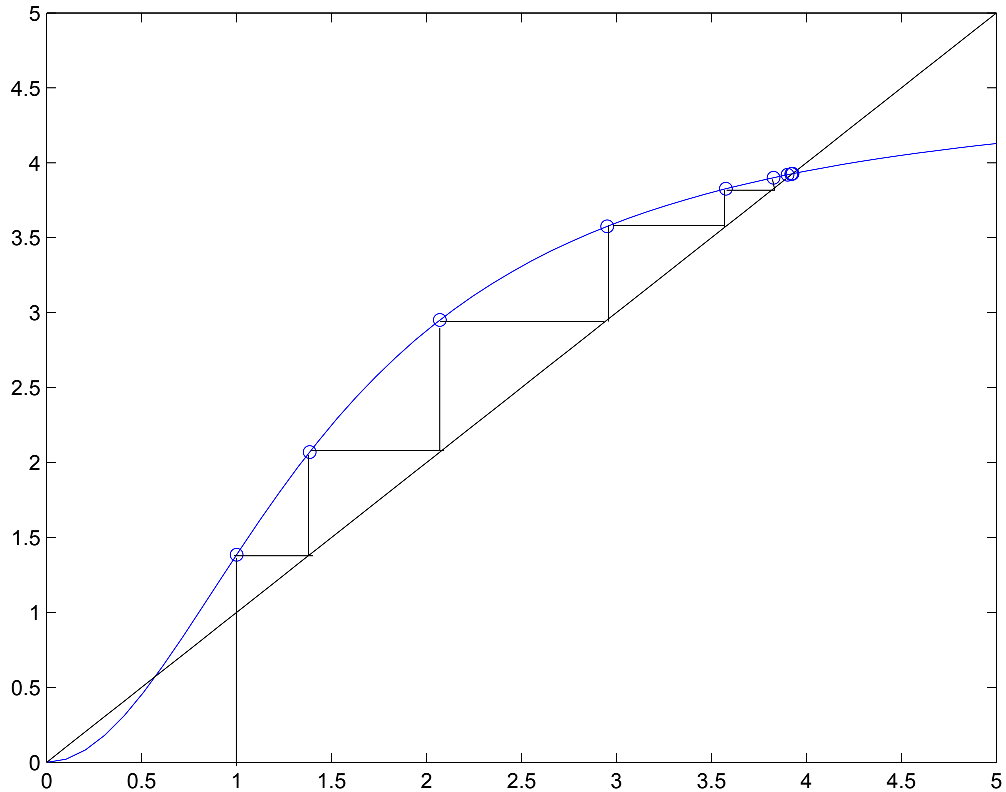
We find the stationary points $\alpha_2 = 1.5$ and $\alpha_3 = 3.9271$.

Function $\phi_2(x)$:



$$
\begin{aligned}
x^{(0)} &= 1.0000, & |x^{(0)} - \alpha_2| &= 0.5000 \\
x^{(1)} &= 1.2000, & |x^{(1)} - \alpha_2| &= 0.3000 \\
x^{(2)} &= 1.3333, & |x^{(2)} - \alpha_2| &= 0.1667 \\
x^{(3)} &= 1.4118, & |x^{(3)} - \alpha_2| &= 0.0882
\end{aligned}
$$

Function $\phi_3(x)$:



$$
\begin{aligned}
x^{(0)} &= 1.0000, & |x^{(0)} - \alpha_3| &= 2.9271 \\
x^{(1)} &= 1.3846, & |x^{(1)} - \alpha_3| &= 2.5424 \\
x^{(2)} &= 2.0703, & |x^{(2)} - \alpha_3| &= 1.8568 \\
x^{(3)} &= 2.9509, & |x^{(3)} - \alpha_3| &= 0.9761
\end{aligned}
$$

Example. 6 (cont) We have used the fixed point algorithms using the two fonctions ϕ_1 and ϕ_2 with initial value $x^{(0)} = 0.7$. Remember that both have the same fixed point α.

$$x = \phi_1(x) = 1 - \sin(2x)$$

$$x = \phi_2(x) = \frac{1}{2}\arcsin(1-x), \qquad 0 \leq x \leq 1$$

```
>>  [p1,res1,niter1]=fixpoint(phi1,0.7,1e-8,1000);
>>  [p2,res2,niter2]=fixpoint(phi2,0.7,1e-8,1000);
```

The fixed point algorithm with the first function does not converge, while with the second one it converges to $\alpha = 0.352288459558650$ in 44 iterations. Indeed, $\phi_1'(\alpha) = -1.5237713$ and $\phi_2'(\alpha) = -0.65626645$.

More about the Newton method.

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,

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

Theorem 1. *If f is twice differentiable, $f(\alpha) = 0$ 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

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

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 2. *Let α be a zero of f. α is said to have multiplicity m, $m \in \mathbb{N}$, if $f(\alpha) = \ldots = f^{(m-1)}(\alpha) = 0$ and $f^{(m)}(\alpha) \neq 0$.*
A zero that has multiplicity $m = 1$ is called simple zero.

Remark 2. *If $f'(\alpha) = 0$, the convergence of the Newton method is linear, not quadratic. We can use the modified Newton method:*

$$x^{(k+1)} = x^{(k)} - m\frac{f(x^{(k)})}{f'(x^{(k)})}, \quad k = 0, 1, 2 \ldots . \tag{7}$$

where m is the multiplicity of α.

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

A stopping criterion for Newton

When to stop the Newton method? A good stopping criterion is the **control of the increment** : the iterations is completed when

$$|x^{(k+1)} - x^{(k)}| < \epsilon \tag{8}$$

where ϵ is a fixed tolerance.

Indeed, if we denote $e^{(k)} = \alpha - x^{(k)}$ is the error of the iteration k, we have

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

where $\xi^{(k)}$ is between $x^{(k)}$ and α, and

$$x^{(k+1)} - x^{(k)} = \alpha - x^{(k)} - \alpha + x^{(k+1)} = e^{(k)} - e^{(k+1)} = \left(1 - \phi'(\xi^{(k)})\right) e^{(k)}. \quad (9)$$

Assuming that if k is large enough, we have $\phi'(\xi^{(k)}) \approx \phi'(\alpha)$ and knowing that the Newton method for $\phi'(\alpha) = 0$, if α is a simple zero, we find the estimation

$$|e^{(k)}| \approx |x^{(k+1)} - x^{(k)}|.$$

The error that we commit when we adopt the criterion (8) is smaller than the fixed tolerance.

Stopping criteria: the general case

In general, for all discussed methods, we can use two different stopping criteria: the iterations is completed when

$$|x^{(k+1)} - x^{(k)}| < \epsilon \qquad \text{(control of the increment)},$$

or

$$|f(x^{(k)})| < \epsilon \qquad \text{(control of the residual)},$$

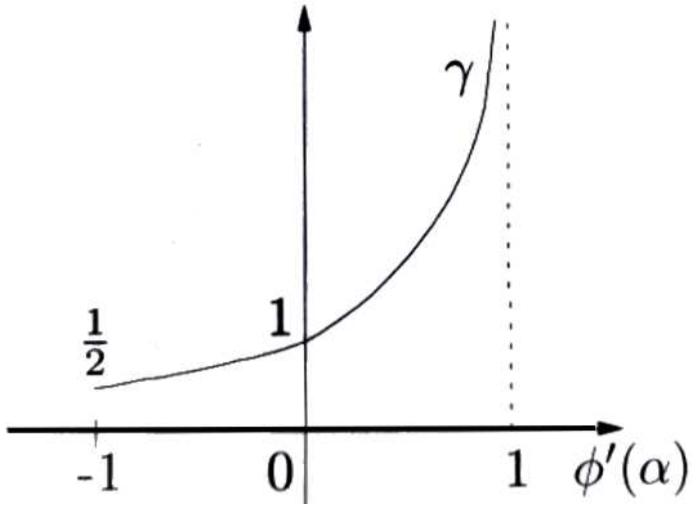
where ϵ is a fixed tolerance.

Using fixed point iterations we obtain the following estimation:

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

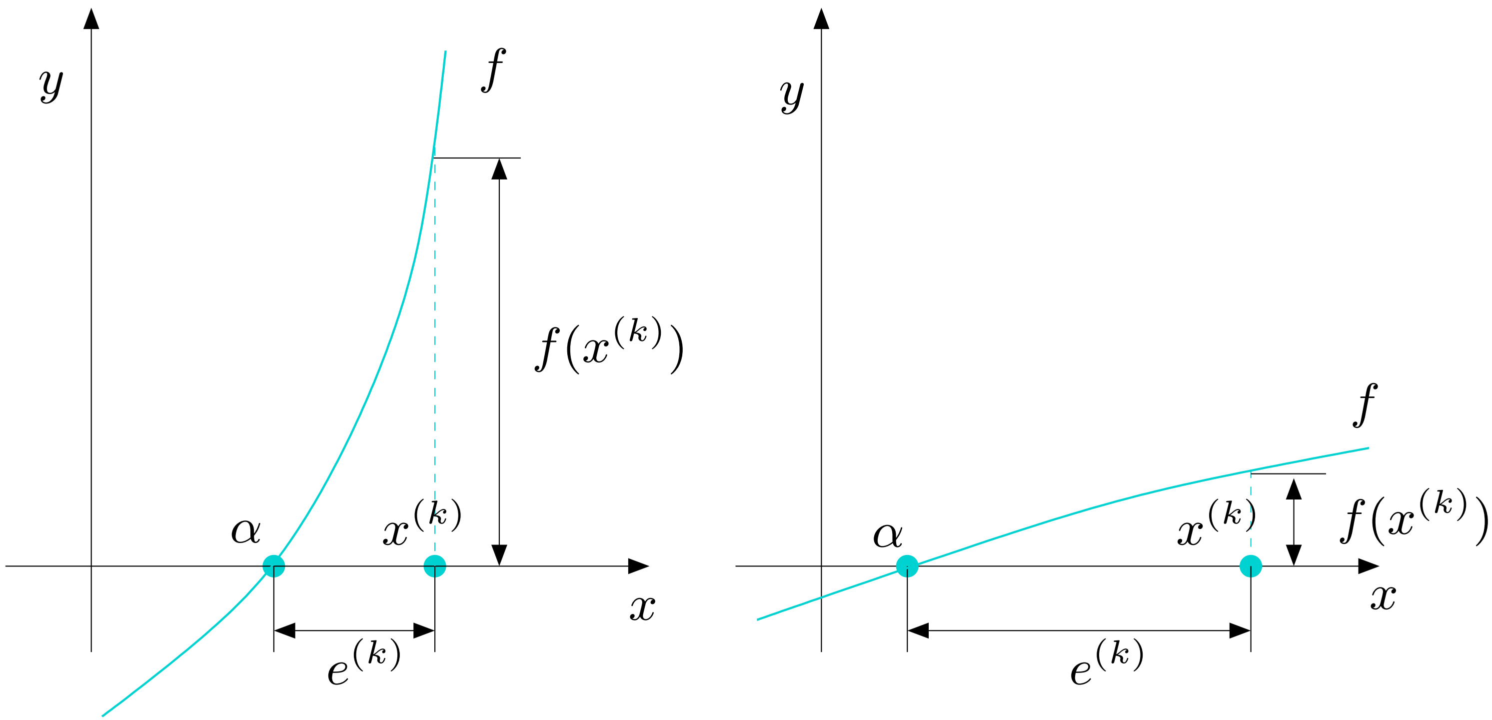
We can plot the graph of $\frac{1}{(1-\phi'(\alpha))}$ and comment on the relevance of the stopping criterium based on the increment:

- if $\phi\prime(\alpha)$ is near to 1 the test is not satisfactory
- for methods of order 2 ($\phi\prime(\alpha) = 0$), the criterium is optimal,
- if $-1 < \phi\prime(\alpha) < 0$ the criterium is still all right.



Stopping Criteria

The stopping criterium based on the control on the residual $|f(x^{(k)})| < \epsilon$ is satisfactory only if $|f'| \simeq 1$ near the root α. Otherwise it is too strong (if $|f'| \gg 1$) or too weak (if $|f'| \ll 1$):

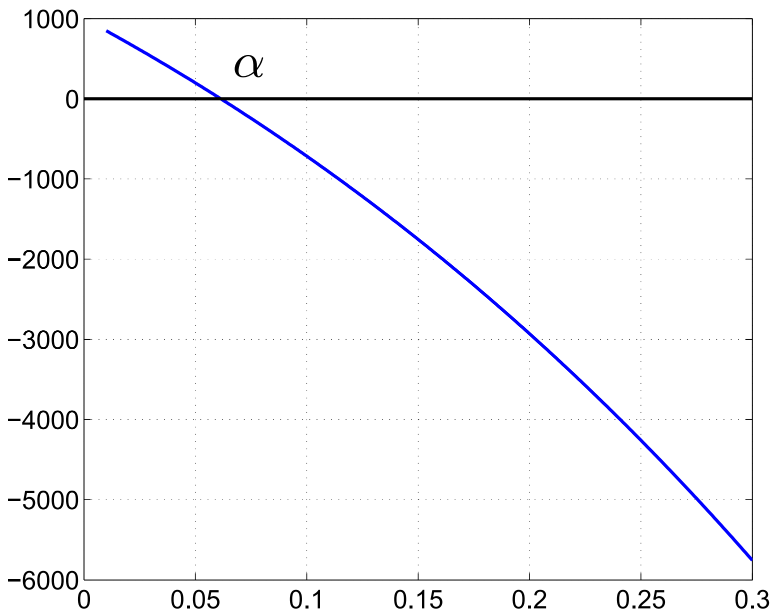


Two cases where the residual is a bad estimator of the error: $|f'(x)| \gg 1$ (left), $|f'(x)| \ll 1$ (right)) with x near to α

Applications

Example. 1 (suite) We draw the graph of $f(I) = M - v\frac{1+I}{I}\left[(1+I)^n - 1\right]$ on the interval $[0.010.3]$ with $M = 6000$, $v = 1000$ and $n = 5$:

```
>> f=@(x) 6000-1000*(1+x).*((1+x).^5 - 1)./x;
>> I = [0.01:0.001:0.3];
>> grid on;plot(I,feval(f,x));
```



The root of f is between 0.05 and 0.1.

We can apply the bisection method on the interval $[0.05, 0.1]$ with a tolerance 10^{-5}

```
>> [zero,res,niter]=bisection(f,0.05,0.1,1e-5,1000);
```

The approximate solution after 12 iterations is $\bar{x} = 0.061407470703125$.

We can apply the Newton method with initial guess $x^{(0)} = 0.05$

```
>> df=@(x) 1000*((1+x).^5.*(1-5*x) - 1)./(x.^2);
>> [zero,res,niter]=newton(f,df,.05,1e-5,1000);
```

The result is approximately the same, but we need only 3 iterations

The interest rate is 6.14%.

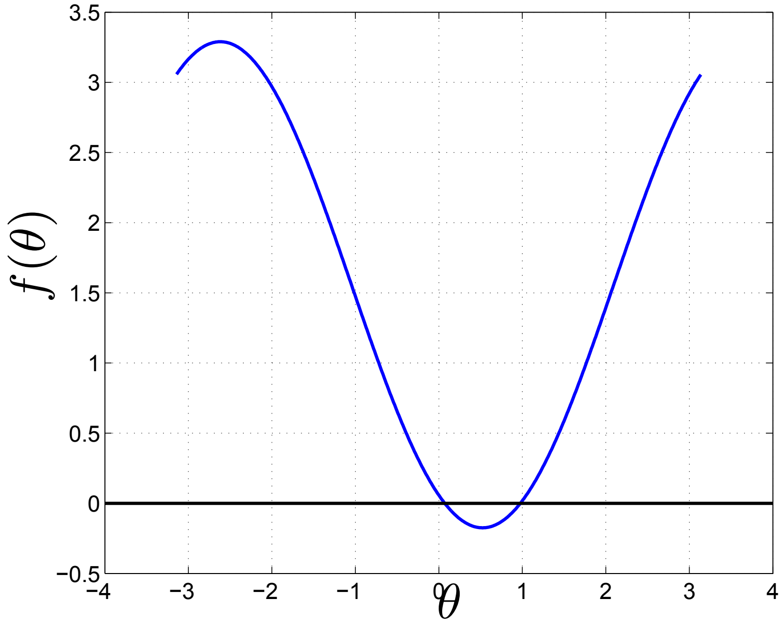
Example. 2 (cont) We would like to plot the angle θ as function of ω for $0 \leq \omega \leq \pi$ with $a_1 = 10\,cm$, $a_2 = 13\,cm$, $a_3 = 8\,cm$, $a_4 = 10\,cm$.
For each ω, we have to solve the nonlinear poblem

$$f(\theta) = \frac{a_1}{a_2} cos(\omega) - \frac{a_1}{a_4} cos(\theta) - cos(\omega - \theta) + \frac{a_1^2 + a_2^2 - a_3^2 + a_4^2}{2 a_2 a_4} = 0. \qquad (10)$$

To start with, we plot the graph of $f(\theta)$ for $\omega = \pi/3$:

```
>> F = @(x, a1, a2, a3, a4, omega) ...
      (a1/a2)*cos(omega) - (a1/a4)*cos(x) - cos(omega-x) ...
    + ( (a1.^2 + a2.^2 - a3.^2 + a4.^2) / (2*a2*a4) );
>> a1=10; a2=13; a3=8; a4=10; omega=pi/3;
>> f = @(x) F(x,a1,a2,a3,a4,omega);
>> x = [-pi:0.01:pi];
>> plot( x, f(x) ); grid on;
```

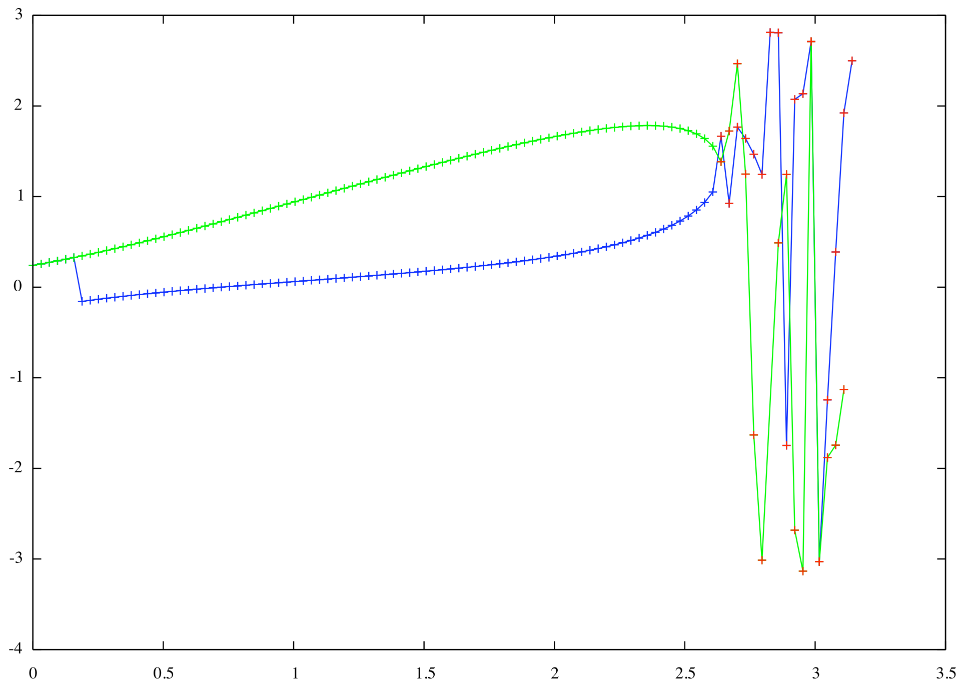
Function f with $\omega = \pi/3$.



We have two roots, which means that we have two possible configurations.

Now we chose 101 different values for ω, $\omega_k = k\frac{\pi}{100}$, $k = 0, \ldots, 100$ and for each of them solve the nonlinear problem (10) with the Newton method. Since we know that we may have two distinct solutions, we give to different initial guesses to our Newton method. For example $\theta_{01} = -0.1$ and $\theta_{02} = 2/3\pi$

The following figure shows the solutions as function of ω.
For $\omega > 2.6358$, the Newton algorithm does not converge anymore. In fact, with these values there is no configuration possible



Here are the Matlab/Octave commands that we have used:

```
>> n=101; x01=-0.1; x02=2*pi/3; nmax=100;
>> dF = @(x,a1,a2,a3,a4,w) a1/a4*sin(x)-sin(w-x);
>> for k=1:1:n
    omega(k) = (k-1)*pi/100;
    f  = @(x)  F(x,a1,a2,a3,a4,omega(k));
    df = @(x) dF(x,a1,a2,a3,a4,omega(k));
    [theta1(k),res,niter] = newton(f,df,x01,1e-5,nmax);
    [theta2(k),res,niter] = newton(f,df,x02,1e-5,nmax);
   end
>> plot(omega,theta1,'b:',omega,theta2,'g-')
```

Example. 3 (suite) We consider the carbon dioxide (CO_2), for which $a = 0.401 \; Pa\, m^6$ and $b = 42.7 \cdot 10^{-6} \; m^3$.

We search the volume occupied by $N = 1000$ molecules of CO_2 in temperature $T = 300 \; K$ and pressure $p = 3.5 \cdot 10^7 \; Pa$. We know that the Boltzmann constant is $k = 1.3806503 \cdot 10^{-23} \; Joule\, K^{-1}$.

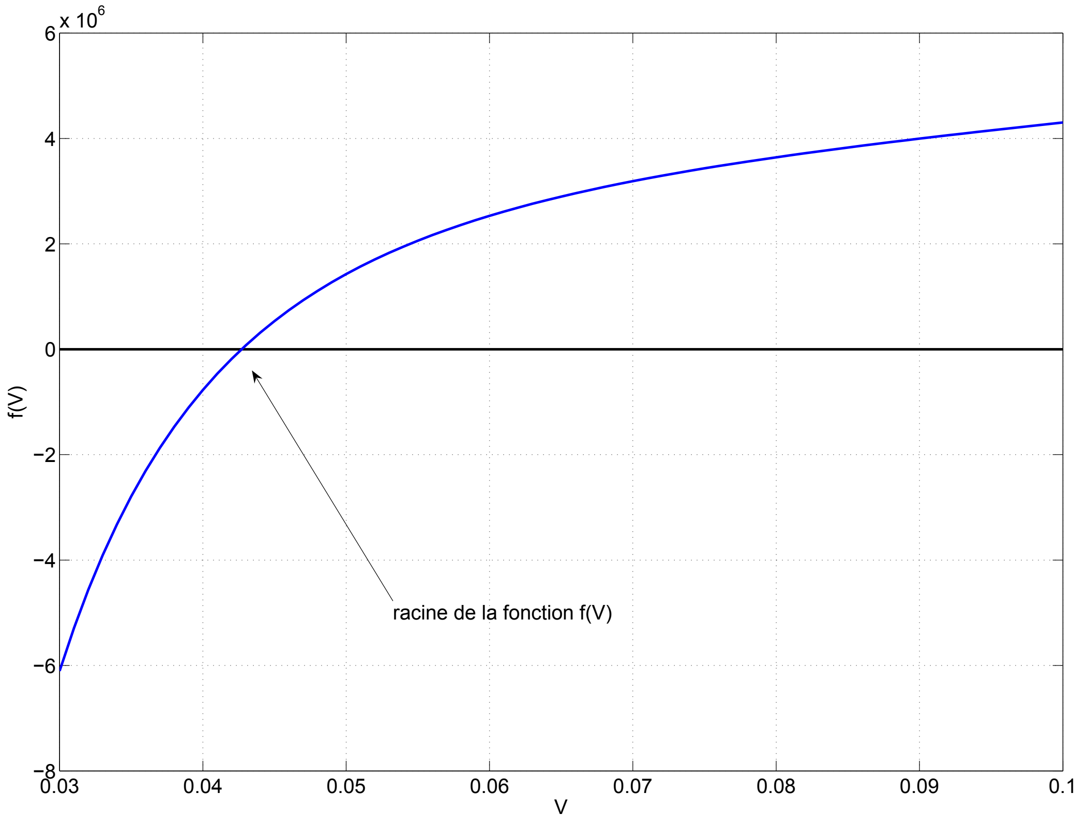
We draw the graph of the function

$$f(V) = \left[p + a\left(\frac{N}{V}\right)^2\right](V - Nb) - kNT$$

for $V > 0$. We do not consider $V < 0$ (it does not have physical meaning), because V is the volume of gas.
We use the commands in Matlab/Octave:

```
>> a=0.401; b=42.7e-6; p=3.5e7; T=300; N=1000; k=1.3806503e-23;
>> f = @(x,p,T,a,b,N,k)(p+a*((N./x).^2)).*(x-N*b)-k*N*T;
>> x=[0.03:0.001:0.1];
>> plot(x,f(x,p,T,a,b,N,k))
>> grid on
```

We obtain the graph of the function $f(V)$:



We see that there is a zero for $0.03 < V < 0.1$. If we apply the bisection method on the interval $[0.03, 0.1]$ with a tolerance 10^{-12}:

```
[zero,res,niter]=bisection(f,0.03,0.1,1e-12,1000,p,T,a,b,N,k);
```

then we find, after 36 iterations, the value $V = 0.0427$.
If we use the Newton method with the same tolerance, starting form the initial point $x^{(0)} = 0.03$,

```
>> df = @(x,p,T,a,b,N,k) -2*a*N^2/(x^3)*(x-N*b)+(p+a*((N./x).^2));
>> [zero,res,niter]=newton(f,df,0.03,1e-12,1000,p,T,a,b,N,k);
```

then we find the same solution after 6 iterations.
The conclusion is that the volume V occupied by the gas is $0.0427\ m^3$.

The rope method

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

$$x^{(k+1)} = x^{(k)} - \frac{1}{q} f(x^{(k)}), \quad k = 0, 1, 2 \ldots. \tag{11}$$

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

Example. 6 (suite) We apply the rope method and the Newton method to find the zero of f.

The rope method in the interval $[-1, 1]$, with $x^{(0)} = 0.7$:

```
>> [zero,res,niter]=chord(f,-1,1,0.7,1e-8,1000)
```

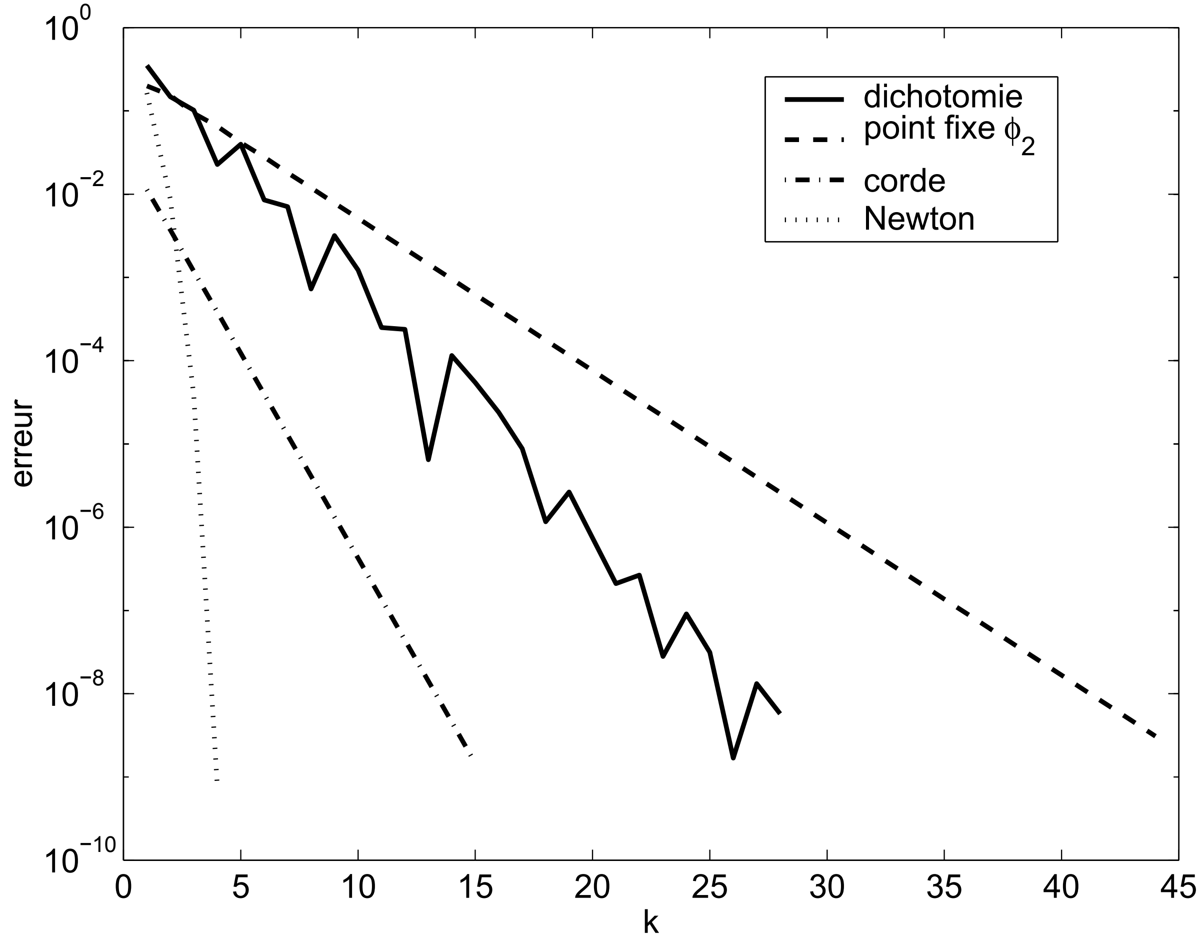
We find the result after 15 iterations.

The Newton method with the same $x^{(0)}$:

```
>> df = @(x) 2*cos(2*x) + 1;
>> [zero,res,niter]=newton(f,df,0.7,1e-8,1000);
```

We find the result after 5 iterations. Much faster.

Values of the errors plotted versus the number of iterations for 4 methods: bisection, fixed point ϕ_2, rope and Newton. There is logarithmic scale on the axis y.



Remark 3. *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:*

$$| 1 - \frac{1}{q} f'(\alpha) | < 1 \, .$$