# Nonlinear equations

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slides based on lecture notes/slides from L. Dede

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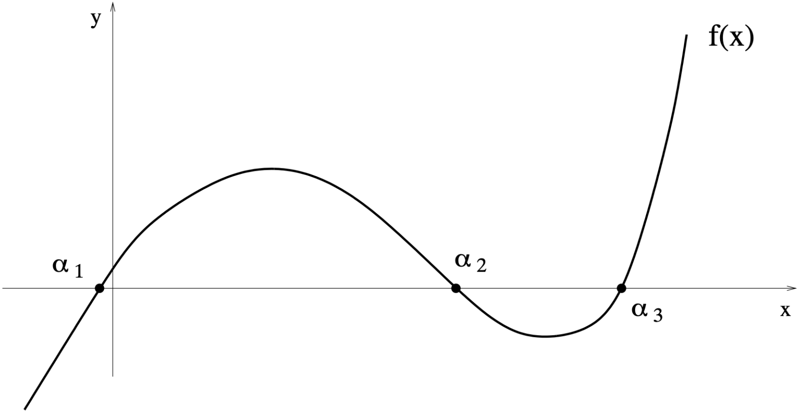
# Plan

# Plan

# Nonlinear Equations

Objective: Approximate numerically the root of scalar (or vector) non-linear function $f(x)$, i.e.
find $\alpha \in \mathbb{R}$ such that $f(\alpha) = 0$ in the interval $I = (a, b) \subseteq \mathbb{R}$



# Examples of nonlinear equations

**Example 1 (Interest rates).** We want to compute the mean interest rate $I$ of a portfolio over several years. We invest $v = 1000\,\text{CHF}$ every year. After 5 years, we end up with $M = 6000\,\text{CHF}$. 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

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

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

# Examples of nonlinear equations

**Example 2 (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 $p$, $V$, and $T$) is:

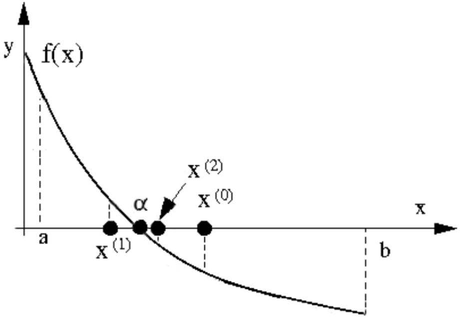
$$\left(p + \frac{aN^2}{V^2}\right)(V - Nb) = kNT,$$

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

# Plan

# Bisection method (book chap 2.1)

- Compute the root of a continuous function $f$, i.e., the point $\alpha$ such that $f(\alpha) = 0$.
- Build a sequence $x^{(0)}, x^{(1)}, \ldots, x^{(k)}$, with $x^{(0)}$ such that $\lim_{k\to\infty} x^{(k)} = \alpha$.

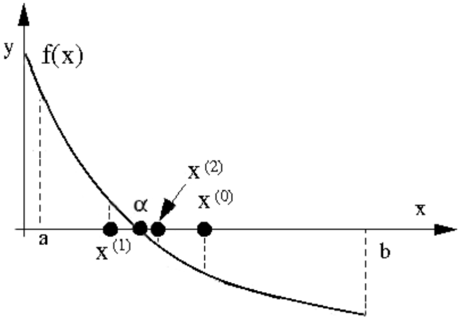


# Foundation of the bisection method

## Theorem 1 (Theorem 2.1 in book)

*Zeros of a continuous function*

*Let $f(x)$ be a continuous function in $I = (a, b)$, that is $f \in C^0([a, b])$. If $f(a)f(b) < 0$, then there exists at least one zero $\alpha \in I$ of the function $f(x)$.*



# Bisection method: algorithm

- Assume there exists an unique zero $\alpha \in (a, b)$ of $f \in C^0([a, b])$ and $f(a)f(b) < 0$
- Search $\alpha$ by recursively approximating it with the sequence of mid-points of subintervals $I^{(k)}$ of $I = (a, b)$ for which $f(x)$ changes sign

# Bisection method: first step

Then start on $I^{(0)} = (a^{(0)}, b^{(0)}) = I = (a, b)$:

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:
   3.1 If $f(x^{(0)})f(a^{(0)}) > 0 \implies$ the zero $\alpha \in (x^{(0)}, b^{(0)})$, and we define:

$$a^{(1)} = x^{(0)}, \quad b^{(1)} = b^{(0)}, \quad x^{(1)} = \frac{a^{(1)} + b^{(1)}}{2}$$

   3.2 If $f(x^{(0)})f(a^{(0)}) < 0 \implies$ the zero $\alpha \in (a^{(0)}, x^{(0)})$, and we define:

$$b^{(1)} = x^{(0)}, \quad a^{(1)} = a^{(0)}, \quad x^{(1)} = \frac{a^{(1)} + b^{(1)}}{2}$$

Continue recursively on $I^{(1)} = (a^{(1)}, b^{(1)}), \ldots I^{(k)} = (a^{(k)}, b^{(k)})$ till convergence.

# Bisection method: first step

Then start on $I^{(0)} = (a^{(0)}, b^{(0)}) = I = (a, b)$:

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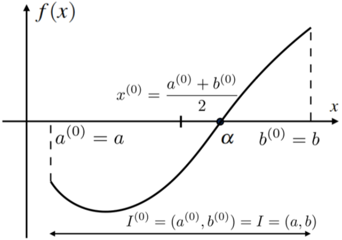
Continue recursively on $I^{(1)} = (a^{(1)}, b^{(1)}), \ldots I^{(k)} = (a^{(k)}, b^{(k)})$ till convergence.

# Bisection method: example

Step 0.

$I^{(0)} = \left(a^{(0)}, b^{(0)}\right) = I = (a,b)$ and

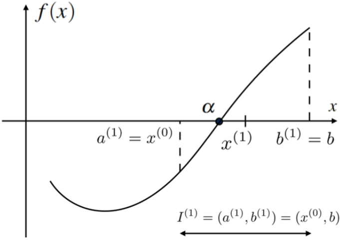
$x^{(0)} = \dfrac{a^{(0)} + b^{(0)}}{2} = \dfrac{a+b}{2}$



# Bisection method: example

Step 1.

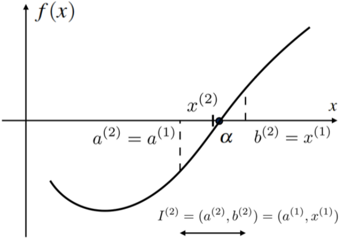
Since $f\left(x^{(0)}\right) f\left(b^{(0)}\right) < 0$:
$a^{(1)} = x^{(0)}$, $b^{(1)} = b$,
$I^{(1)} = (a^{(1)}, b^{(1)}) = (x^{(0)}, b)$, and
$x^{(1)} = \dfrac{a^{(1)} + b^{(1)}}{2} = \dfrac{x^{(0)} + b}{2}$.



# Bisection method: example

Step 2.

Since $f\left(x^{(1)}\right) f\left(a^{(1)}\right) < 0$:
$a^{(2)} = a^{(1)}$, $b^{(2)} = x^{(1)}$,
$I^{(2)} = (a^{(2)}, b^{(2)}) = (a^{(1)}, x^{(1)})$, and
$x^{(2)} = \dfrac{a^{(2)} + b^{(2)}}{2} = \dfrac{a^{(1)} + x^{(1)}}{2}$.



# Computational error of the bisection method

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

$$|I^{(k)}| := b^{(k)} - a^{(k)} \equiv \frac{|I^{(k-1)}|}{2} \quad \text{for all} \quad k \geq 1,$$

$$|I^{(k)}| = \frac{|I^{(0)}|}{2^k} = \frac{b-a}{2^k} \quad \text{for all} \quad k \geq 0.$$

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# Bounding the computational error

Define computational error as

$$e^{(k)} = |x^{(k)} - \alpha|$$

and the error estimator as

$$\tilde{e}^{(k)} := |I^{(k+1)}| = \frac{b-a}{2^{k+1}}$$

# Bounding the computational error

We have:

$$e^{(k)} \leq \tilde{e}^{(k)} := |I^{(k+1)}| = \frac{b-a}{2^{k+1}} \quad \text{for all} \quad k \geq 0. \tag{2.1}$$

This implies that the bisection method is convergent; indeed

$$\lim_{k \to +\infty} e^{(k)} = 0$$

since $e^{(k)} \leq \tilde{e}^{(k)}$ for all $k \geq 0$ and

$$\lim_{k \to +\infty} \tilde{e}^{(k)} = \lim_{k \to +\infty} \frac{b-a}{2^{k+1}} = 0.$$

# Convergence order

## Definition 2 (Definition 2.1 in book)

An iterative method for the approximation of the zero $\alpha$ of the function $f(x)$ is convergent with order $p$ if and only if

$$\lim_{k \to +\infty} \frac{|x^{(k+1)} - \alpha|}{|x^{(k)} - \alpha|^p} = \mu, \tag{1}$$

with $\mu > 0$ a real number independent of $k$, which is called the asymptotic convergence factor. In the case of linear convergence, i.e., for $p = 1$, we need $0 < \mu < 1$.

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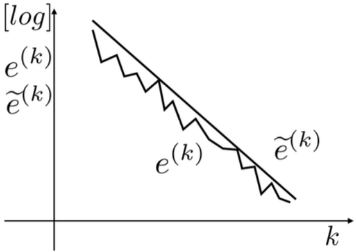
# No convergence order for bisection method

- The error may not be monotonically convergent, i.e., it is possible that $e^{(k+1)} > e^{(k)}$ for some $k \geq 0$;
- A convergence order cannot be established according to Eq. (1)

The sequence of error estimators $\{\tilde{e}^{(k)}\}$ is linearly convergent according to Eq. (1) with $p = 1$ and $\mu = \frac{1}{2}$; indeed:

$$\frac{\tilde{e}^{(k+1)}}{\tilde{e}^{(k)}} = \frac{(b-a)/2^{k+2}}{(b-a)/2^{k+1}} = \frac{1}{2} \quad \text{for all} \quad k \geq 0.$$



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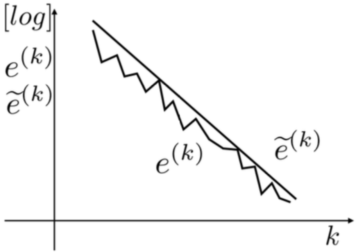


# Algorithm of bisection method

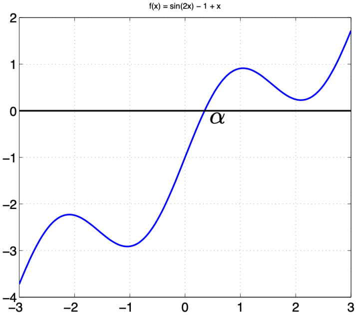
**Algorithm 1** Bisection Method

**Require:** $f$, $a$, $b$, tol, $k_{\max}$
**Assert:** $\alpha$

Set $k = 0$, $a^{(0)} = a$, $b^{(0)} = b$, $x^{(0)} = \frac{a+b}{2}$, $ee^{(0)} = \frac{b-a}{2}$
**while** $\tilde{e}^{(k)} >$ tol **and** $k < k_{\max}$ **do**
    **if** $f(x^{(k)}) = 0$ **then**
        Set $\alpha = x^{(k)}$
        **return**
    **else if** $f(a^{(k)})f(x^{(k)}) < 0$ **then**
        Set $a^{(k+1)} = a^{(k)}$, $b^{(k+1)} = x^{(k)}$
    **else if** $f(b^{(k)})f(x^{(k)}) < 0$ **then**
        Set $a^{(k+1)} = x^{(k)}$, $b^{(k+1)} = b^{(k)}$
    **end if**
    Set $x^{(k+1)} = \frac{a^{(k+1)} + b^{(k+1)}}{2}$
    Set $\tilde{e}^{(k+1)} = \frac{b^{(k+1)} - a^{(k+1)}}{2}$
    Set $k = k + 1$
**end while**
Set $\alpha = x^{(k)}$

# Bisection method: example

**Example 3.** We want to find the zero of the function
$f(x) = \sin(2x) - 1 + x$.
We draw the graph of the function $f$ using Matlab

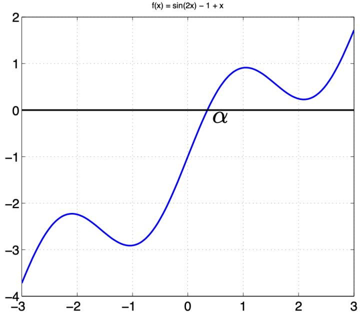


# Bisection method: example

If we apply the bisection method in the interval $[-1, 1]$ with a tolerance of $10^{-8}$ and a maximum number of iterations $k_{\max} = 1000$, using the following command in Matlab:

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

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



# Plan

Numerical solution of a non-linear equation

Bisection method

Newton method

- Convergence
- Modified Newton method
- Stopping criterion and algorithm
- Inexact and quasi-Newton methods

Fixed point iterations

# Newton method (book, chap 2.2)

Let $f : \mathbb{R} \to \mathbb{R}$, $f \in C^0(I)$, be a differentiable function in $I = (a, b)$.
Let $x^{(0)}$ be an initial guess. Consider the equation of the tangent line to the curve $(x, f(x))$ at coordinate $x^{(k)}$ and with slope $f'(x^{(k)})$:

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

Newton method searches the new iterate $x^{(k+1)}$ at the intersection between the tangent line and the $x$-axis, i.e.,

$$y(x^{(k+1)}) = 0.$$

We deduce the Newton iterate:

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

provided $f'(x^{(k)}) \neq 0$ for all $k \geq 0$.

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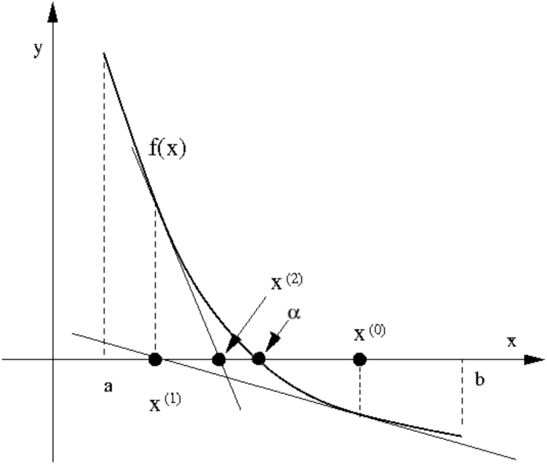
# Newton method

Starting from the point $x^{(0)}$, the root of $f$ is obtained as the limit of the sequence $\{x^{(k)}\}_{k=0}^{\infty}$.



# Newton method: algorithm

**Algorithm 2** Newton Method

**Require:** $f$, $x^{(0)}$, tol, $k_{\text{max}}$

**Assert:** $\alpha$

1: Set $k = 0$
2: **while** stopping criterion is false **do**
3: Set $x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$
4: Set $k = k + 1$
5: **end while**
6: Set $\alpha = x^{(k)}$

# Newton method and Taylor expansion

Assume $f \in C^2(I)$, then the Taylor expansion of $f(x)$ around $x^{(k)}$ is:

$$f\left(x^{(k+1)}\right) = f\left(x^{(k)}\right) + f'\left(x^{(k)}\right)(x^{(k+1)} - x^{(k)}) + O\left((x^{(k+1)} - x^{(k)})^2\right)$$

If $f\left(x^{(k+1)}\right) = 0$, then the Newton method is the first-order approximation of the Taylor expansion of $f(x)$ around $x^{(k)}$;
in order to satisfy this assumption, one needs $x^{(k+1)} - x^{(k)}$ to be "small."

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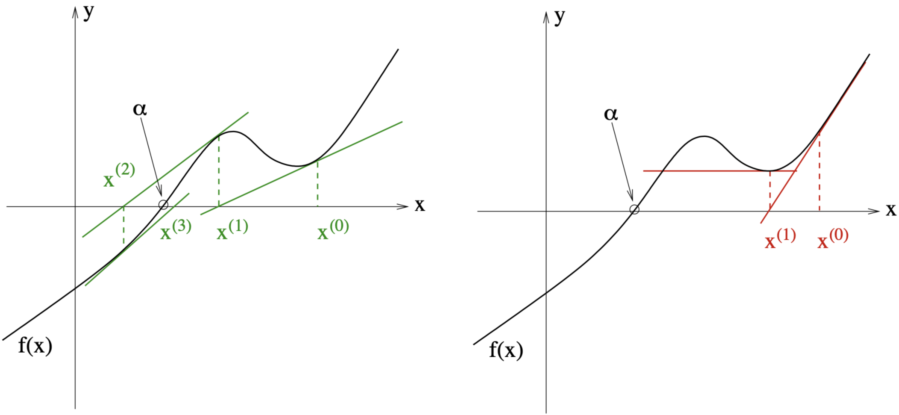
# Convergence

Does this method always converge?

- it depends on the property of the function;
- and on the initial guess $x^{(0)}$ (should be "sufficiently" close to the zero $\alpha$).



# Convergence of the Newton method

## Proposition 3 (Proposition 2.2 in book)

*If*

- $f \in C^1(I)$,
- $x^{(0)}$ *is "sufficiently" close to* $\alpha \in I$, *and*
- $f'(\alpha) \neq 0$,

*then the Newton method is convergent to* $\alpha$, *provided that* $f'(x^{(k)}) \neq 0$ *for all* $k \geq 0$.

# Convergence order of the Newton method

## Proposition 4 (Proposition 2.3 in book)

*Let $I_\alpha$ be a neighborhood of $\alpha$. If $f \in C^2(I_\alpha)$, $x^{(0)}$ is "sufficiently" close to $\alpha$, and $f'(\alpha) \neq 0$, then the Newton method is convergent with order 2 (quadratically) to $\alpha$, provided that $f'(x^{(k)}) \neq 0$ for all $k \geq 0$. We have:*

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

*following Eq. (1), $p = 2$ is the convergence order and $\mu = \frac{1}{2}\frac{f''(\alpha)}{f'(\alpha)}$ is the asymptotic convergence factor.*

## Proof.

*Interpretation as a fixed point iterations method, next lecture !* □

# Zero multiplicity

## Definition 5 (Definition 2.2 in book)

Let $f \in C^m(I_\alpha)$, with $m \in \mathbb{N}$ such that $m \geq 1$.

The zero $\alpha \in I_\alpha$ is said to be of multiplicity $m$ if $f^{(i)}(\alpha) = 0$ for all $i = 0, \ldots, m-1$ and $f^{(m)}(\alpha) \neq 0$.

If $m = 1$, the zero $\alpha$ is called simple; otherwise, it is called multiple.

# Zero multiplicity

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# Convergence order of Newton, zero multiple

### Proposition 6 (Proposition 2.4 in book)

*If $f \in C^2(I_\alpha) \cap C^m(I_\alpha)$ and $x^{(0)}$ is "sufficiently" close to the zero $\alpha$ of multiplicity $m > 1$, then the Newton method is convergent with order 1 (linearly) to $\alpha$, provided that $f'(x^{(k)}) \neq 0$ for all $k \geq 0$. In particular, following Eq. (1), we have:*

$$\lim_{k \to +\infty} \frac{|x^{(k+1)} - \alpha|}{|x^{(k)} - \alpha|} = \mu,$$

*with $p = 1$ being the convergence order and $\mu \in (0, 1)$ the asymptotic convergence factor.*

# Modified Newton method

- Assume $f \in C^m(I_\alpha)$, with $\alpha \in I_\alpha$ and $m \geq 1$ the multiplicity of $\alpha$.
- The modified Newton iterate is:

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

  provided $f'(x^{(k)}) \neq 0$ for all $k \geq 0$.
- Requires knowledge or estimation of the multiplicity $m$

# Convergence order of modified Newton method

## Proposition 7 (Proposition 2.5 in book)

*If $f \in C^2(I_\alpha) \cap C^m(I_\alpha)$, with $m \geq 1$ the multiplicity of the zero $\alpha \in I_\alpha$, and $x^{(0)}$ is "sufficiently" close to $\alpha$,*

*then modified Newton is convergent with order 2 to $\alpha$, provided that $f'(x^{(k)}) \neq 0$ for all $k \geq 0$.*

# Stopping criterion for Newton

- Since $\alpha$ is unknown, the error $e^{(k)} = |x^{(k)} - \alpha|$ is also unknown $\implies$ need to use estimators
- Criterion based on difference of succesive iterates (discuss next lecture) stop algorithm when $\tilde{e}^{(k)} < tol$, where

$$\tilde{e}^{(k)} = \begin{cases} |\delta^{(k-1)}| & \text{if } k > 0 \\ \text{tol} + 1 & \text{if } k = 0 \end{cases} \quad \text{with } \delta^{(k)} := x^{(k+1)} - x^{(k)} \quad \text{for } k \geq 0.$$

- Criterion based on residual

$$\tilde{e}^{(k)} = |r^{(k)}| \quad \text{with } r^{(k)} := f(x^{(k)}), \quad \text{for } k \geq 0$$

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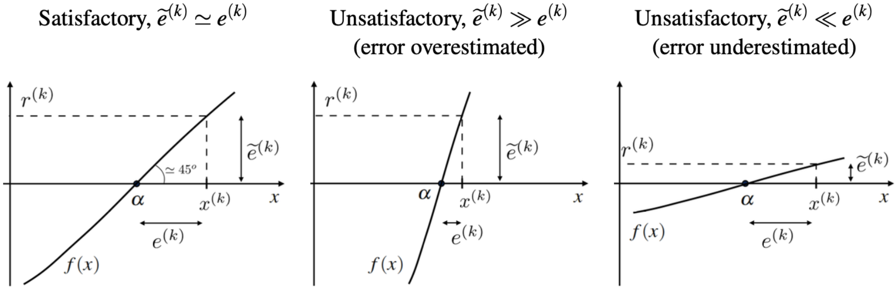

# Newton method: algorithm

**Algorithm 3** Newton's Method

**Require:** $f$, $x^{(0)}$, tol, $k_{\text{max}}$
**Assert:** $\alpha$

```
Set k = 0, ẽ^(0) = tol + 1
while ẽ^(k) > tol and k < k_max do
    Set x^(k+1) = x^(k) − f(x^(k)) / f'(x^(k))
    Set ẽ^(k+1) = |x^(k+1) − x^(k)|
    Set k = k + 1
end while
Set α = x^(k)
```

# Quasi-Newton methods

- Approximate $f'\left(x^{(k)}\right)$ by computationally feasible $q^{(k)} \approx f'\left(x^{(k)}\right)$.
- Quasi-Newton iterate is

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

- Rope method:

$$q^{(k)} = \frac{f(b) - f(a)}{b - a}, \text{for all } k \geq 0, \alpha \in (a, b)$$

- Secant method (order of convergence $p = 1.6$ if zero $\alpha$ is simple):

$$q^{(k)} = \frac{f(x^{(k)}) - f(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}, \text{for all } k \geq 1$$

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- Quasi-Newton iterate is

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

  - Rope method:

$$q^{(k)} = \frac{f(b) - f(a)}{b - a}, \text{for all } k \geq 0, \alpha \in (a, b)$$

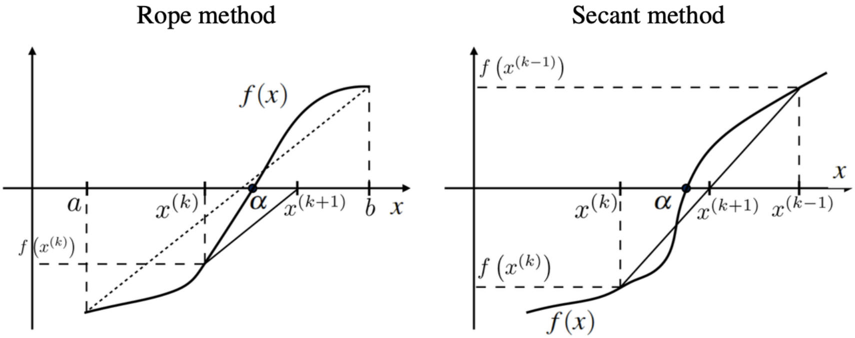
  - Secant method (order of convergence $p = 1.6$ if zero $\alpha$ is simple):

$$q^{(k)} = \frac{f(x^{(k)}) - f(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}, \text{for all } k \geq 1$$

# Rope and secant method at iterate $x^{(k)}$

$$q^{(k)} = \frac{f(b) - f(a)}{b - a}, \qquad q^{(k)} = \frac{f(x^{(k)}) - f(x^{(k-1)})}{x^{(k)} - x^{(k-1)}},$$

for all $k \geq 0, \alpha \in (a, b)$      for all $k \geq 1$



# Plan

Numerical solution of a non-linear equation

Bisection method

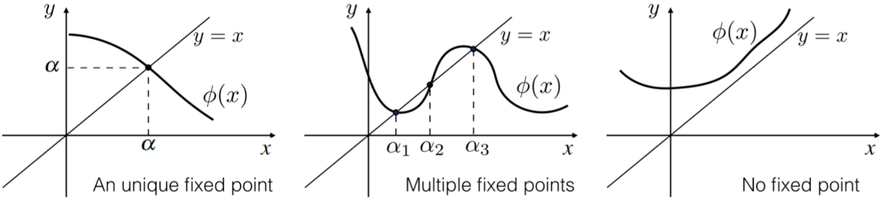
Newton method

Fixed point iterations

- Global convergence in an interval
- Local convergence in a neighborhood of $\alpha$
- Stopping criterion for fixed point iterations
- Newton method as a fixed point iterations method
- Examples and their numerical solution
- Modified Newton method

# Fixed point of a function

**Definition 2.4:** Given the iteration function $\phi : [a, b] \subseteq \mathbb{R} \to \mathbb{R}$, we say that $\alpha \in \mathbb{R}$ is a fixed point of $\phi$ if and only if $\phi(\alpha) = \alpha$.



# Fixed point iterations (chap 2.3 in book)

Find the roots of nonlinear $f(x) = 0$ by solving the equivalent problem:

$$\phi : [a, b] \to \mathbb{R}. \quad x - \phi(x) = 0,$$

where $\phi$ must have the following property:

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

$\implies$ Search for zeros of $f$ by determining the fixed points of $\phi$

**Idea:** It could be computed by the following algorithm:

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

Indeed, if $x^{(k)} \to \alpha$ and if $\phi$ is continuous on $[a, b]$, then the limit $\alpha$ satisfies $\phi(\alpha) = \alpha$.

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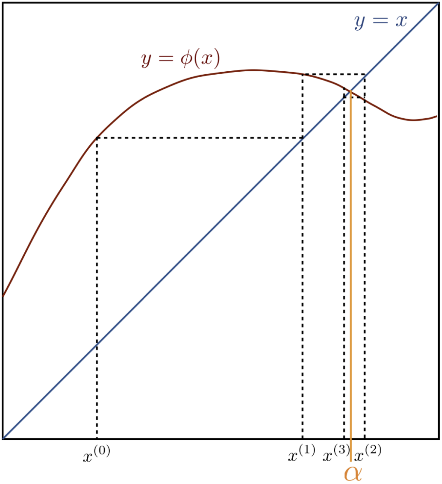
$$x^{(k+1)} = \phi(x^{(k)}), \quad k \geq 0.$$

Indeed, if $x^{(k)} \to \alpha$ and if $\phi$ is continuous on $[a, b]$, then the limit $\alpha$ satisfies $\phi(\alpha) = \alpha$.

# Fixed point iterations (example)

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



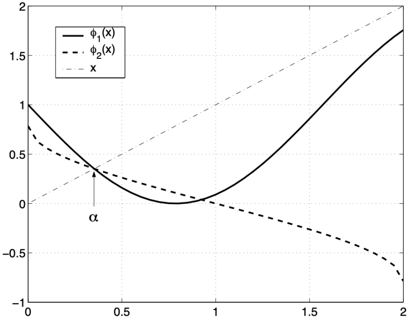
# Example

Consider $f(x) = \sin(2x) - 1 + x = 0$. We can rewrite it in two different fashions. Using $f(\alpha) + \alpha = \alpha$,

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

or setting $f(x) = 0$,

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



# Global convergence in an interval

## Proposition 8 (Proposition 2.7)

*Consider iteration function $\phi : \mathbb{R} \to \mathbb{R}$ and the fixed point iterations.*

1. *If $\phi \in C^0([a, b])$ and $\phi(x) \in [a, b]$ for all $x \in [a, b]$, then there exists at least one fixed point $\alpha \in [a, b]$ of $\phi(x)$.*
2. *If, in addition, $\exists L \in [0, 1)$ s.t.*

$$|\phi(x_1) - \phi(x_2)| \leq L|x_1 - x_2|$$

*for all $x_1, x_2 \in [a, b]$, then the fixed point $\alpha$ is unique in $[a, b]$ and the fixed point iterations algorithm converges, for all the initial guesses $x^{(0)} \in [a, b]$:*

$$\lim_{k \to +\infty} x^{(k)} = \alpha$$

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$$\lim_{k \to +\infty} x^{(k)} = \alpha$$

# Proof of Proposition 2.7

**1. Existence** Consider the function $g(x) = \phi(x) - x$
Since $\phi(x) \in [a, b]$ for all $x \in [a, b]$, we have $g(a) = f(a) - a \geq 0$ and $g(b) = f(b) - b \leq 0$, for which $g(a)g(b) \leq 0$.
By applying the theorem of zeros of a continuous function, there exists at least a zero $\alpha$ of $g(x)$ in $[a, b]$; i.e. $\phi$ has at least one fixed point in $[a, b]$.

**2. Uniqueness** Indeed should two different fixed points exist, $\alpha_1$ and $\alpha_2$, 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 $\phi$

# Proof of Proposition 2.7 (contd)

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

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

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

# Global convergence in an interval

## Proposition 9 (Proposition 2.8)

*If $\phi \in C^1([a,b])$, $\phi(x) \in [a,b]$ for all $x \in [a,b]$, and*

$$|\phi'(x)| < 1 \quad \textit{for all} \quad x \in [a,b],$$

*then there exists a unique fixed point $\alpha \in [a,b]$, and the fixed point iterations method converges for all $x^{(0)} \in [a,b]$ with at least linear order (i.e., order 1), that is:*

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

*with $\phi'(\alpha)$ being the asymptotic convergence factor.*

**Note:** If $0 < |\phi'(\alpha)| < 1$, then for any constant $C$ s.t. $|\phi'(\alpha)| < C < 1$, if k is large enough, we have:

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

# Global convergence in an interval

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*then there exists a unique fixed point $\alpha \in [a, b]$, and*
*the fixed point iterations method converges for all $x^{(0)} \in [a, b]$ with at least linear order (i.e., order 1), that is:*

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

# Local convergence in a neighborhood of $\alpha$

Theorem 10 (Theorem 2.9)

**Lagrange Mean Value Theorem.** *If the function $g \in C^1([a, b])$, then there exists $\xi \in (a, b)$ such that*

$$g(a) - g(b) = g'(\xi)(a - b).$$

# Local convergence in a neighborhood of $\alpha$

**Proposition 2.10 — Ostrowski, local convergence in a neighborhood of the fixed point.** If $\phi \in C^1(I_\alpha)$, with $I_\alpha$ a neighborhood of the fixed point $\alpha$ of $\phi(x)$, and

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

then, if the initial guess $x^{(0)}$ is "sufficiently" close to $\alpha$, the fixed point iterations method converges with at least linear order (i.e., order 1), that is:

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

with $\phi'(\alpha)$ being the asymptotic convergence factor.

# Proof

We only show that the method is at least linearly convergent.
Lagrange Theorem 2.9: there exists $\xi^{(k)} \in (a, x^{(k)})$ s.t.

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

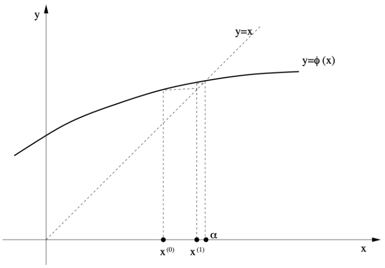
If $\lim_{k\to+\infty} x^{(k)} = \alpha$, then also $\lim_{k\to+\infty} \xi^{(k)} = \alpha$, and hence

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

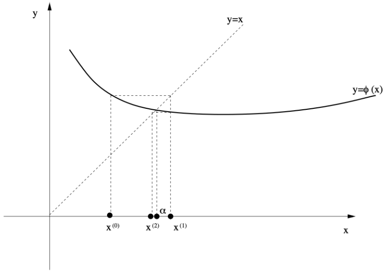
# Examples

Some examples on how the value $\phi'(\alpha)$ influences the convergence.
Convergent cases:

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



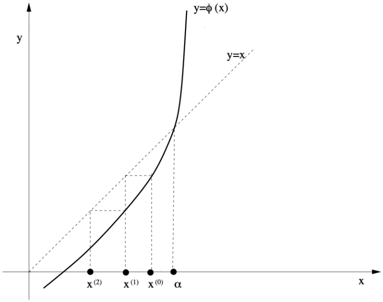

$$-1 < \phi'(\alpha) < 0.$$

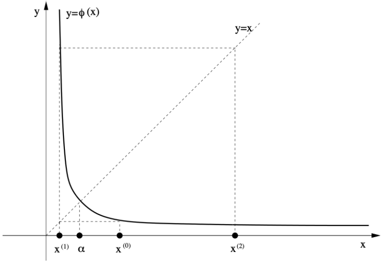


# Examples

Some examples on how the value $\phi'(\alpha)$ influences the convergence.
Divergent cases:

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



- If $|\phi'(\alpha)| < 1$ and $x^{(0)}$ is "sufficiently" close to $\alpha$,
  the method converges to $\alpha$ with at least linear order
- If $|\phi'(\alpha)| = 1$
  the method may either converge or diverge
- If $|\phi'(\alpha)| > 1$ and $x^{(0)} \neq \alpha$,
  the convergence of the method to $\alpha$ is impossible

# Local convergence in a neighborhood of the fixed point

## Proposition 11 (Proposition 2.11 in book)

*If $\phi \in C^2(I_\alpha)$, with $I_\alpha$ a neighborhood of the fixed point $\alpha$ of $\phi(x)$, $\phi'(\alpha) = 0$, and $\phi''(\alpha) \neq 0$, then, if the initial guess $x^{(0)}$ is "sufficiently" close to $\alpha$, the fixed point iterations method converges with order 2,*

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

*with $\frac{1}{2}\phi''(\alpha)$ being the asymptotic convergence factor.*

Proof: Using the Taylor series for $\phi$ with $x = \alpha$, we have

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

where $\xi$ is between $x^{(k)}$ and $\alpha$. So, we have

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

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

# Generalization of the result

## Proposition 12 (Proposition 2.12 in book)

*If $\phi \in C^p(I_\alpha)$ for $p > 1$, with $I_\alpha$ a neighborhood of the fixed point $\alpha$ of $\phi(x)$, $\phi^{(i)}(\alpha) = 0$ for all $i = 1, \ldots, p-1$, and $\phi^{(p)}(\alpha) \neq 0$, then, if the initial guess $x^{(0)}$ is "sufficiently" close to $\alpha$, the fixed point iterations method converges with order $p$, that is:*

$$\lim_{k \to +\infty} \frac{x^{(k+1)} - \alpha}{\left(x^{(k)} - \alpha\right)^p} = \frac{1}{p!}\phi^{(p)}(\alpha),$$

*with $\frac{1}{p!}\phi^{(p)}(\alpha)$ being the asymptotic convergence factor.*

# Example

Consider $f(x) = \sin(2x) - 1 + x = 0$. We have used the fixed point algorithms using the two functions $\phi_1$ and $\phi_2$ with initial value $x^{(0)} = 0.7$. Remember that both have the same fixed point $\alpha$.

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

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

```
>> [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 $\phi_2'(\alpha) = -0.65626645$.

# Stopping criterion for fixed point iterations

- Estimate the error $e^{(k)} = |x^{(k)} - \alpha|$ by the difference of succesive iterates stop algorithm when $\tilde{e}^{(k)} < tol$, where

$$\tilde{e}^{(k)} = \begin{cases} |\delta^{(k-1)}| & \text{if } k \geq 1 \\ \text{tol} + 1 & \text{if } k = 0 \end{cases} \quad \text{with } \delta^{(k)} := x^{(k+1)} - x^{(k)} \quad \text{for } k \geq 0.$$

- If $\phi \in C^1(I_\alpha)$, by Lagrange Mean Value Theorem,

$\exists \xi^{(k)}$ between $x^{(k)}$ and $\alpha$ s.t. $x^{(k+1)} - \alpha = \phi(x^{(k)}) - \phi(\alpha) = \phi'(\xi^{(k)})(x^{(k)} - \alpha)$

- We also have:

$$x^{(k+1)} - \alpha = x^{(k+1)} - x^{(k)} + x^{(k)} - \alpha = \delta_k + x^{(k)} - \alpha$$

- We obtain

$$x^{(k)} - \alpha = -\frac{1}{1 - \phi'(\xi^{(k)})}\delta_k$$

# Stopping criterion for fixed point iterations

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

In a neighbourhood of $\alpha$, $\phi'(\xi^{(k)}) \approx \phi'(\alpha)$

- if $\phi'(\alpha)$ is near to 1, the test is not satisfactory since $e^{(k)} \ll \tilde{e}^{(k+1)}$
- if $\phi'(\alpha) = 0$, the criterion is optimal (second order methods)
- if $\phi'(\alpha) \approx 0$, the criterion is satisfactory

# Newton method as a fixed point iterations method

Consider the iterate of the Newton method

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

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

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

We deduce properties of the Newton method from those of $\phi_N(x)$

## Proposition 13 (Proposition 2.13 in book)

*If $f \in C^m(I_\alpha)$, with $I_\alpha$ a neighborhood of the zero a and $m-1$ the multiplicity of $\alpha$, for the iteration function $x_N(x)$ of Eq. (2.8), we have*

$$\phi'_N(\alpha) = 1 - \frac{1}{m}.$$

**Proof.** The proof is reported in Exercises Series 4

# Convergence of Newton method, $\alpha$ simple zero

For Newton, the zero $\alpha \in I_\alpha$ is said to be of multiplicity $m$ if $f^{(i)}(\alpha) = 0$ for all $i = 0, \ldots, m-1$ and $f^{(m)}(\alpha) \neq 0$.

If $m = 1$, $f(\alpha = 0)$, and $f'(\alpha) \neq 0$, the zero $\alpha$ is called simple; otherwise, it is called multiple.
**Remark 2.14** From Proposition 2.13, if $\alpha$ is a simple zero ($m = 1$), we have

$$\phi_N'(\alpha) = 1 - \frac{1}{m} = 1 - 1 = 0.$$

# Convergence of Newton method, $\alpha$ simple zero

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**Remark 2.14** From Proposition 2.13, if $\alpha$ is a simple zero ($m = 1$), we have

$$\phi_N'(\alpha) = 1 - \frac{1}{m} = 1 - 1 = 0.$$

# Convergence of Newton method, $\alpha$ simple zero

## Corollary 14 (Corollary 2.14 from book)

*If $f \in C^2(I_\alpha)$, $\alpha$ is a simple zero ($m = 1$), and $x^{(0)}$ is "sufficiently" close to $\alpha$, then the Newton method converges with order 2 (quadratically). Indeed:*

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

*where $f_N''(\alpha)$ is the second derivative of the Newton iteration function at $\alpha$.*

## Proof.

*Considering $\phi_N(x) = x - \frac{f(x)}{f'(x)}$, apply Propositions 2.11, 2.12, and Proposition 2.13.* □

# Convergence of Newton method, multiplicity $m > 1$

## Corollary 15 (Corollary 2.15 from book)

*If $f \in C^m(I_\alpha)$, $\alpha$ is a zero of multiplicity $m > 1$, and $x^{(0)}$ is "sufficiently" close to $\alpha$, then the Newton method converges with order 1 (linearly),*

$$\lim_{k \to +\infty} \frac{x^{(k+1)} - \alpha}{x^{(k)} - \alpha} = \phi_N'(\alpha) = 1 - \frac{1}{m} \neq 0.$$

## Proof.

*Considering $\phi_N(x) = x - \frac{f(x)}{f'(x)}$, apply Proposigtion 2.10 and Proposition 2.13.* □

# Examples of nonlinear equations

**Example 1 (Interest rates).** We want to compute the mean interest rate $I$ of a portfolio over several years. We invest $v = 1000\,\text{CHF}$ every year. After 5 years, we end up with $M = 6000\,\text{CHF}$. 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

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

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

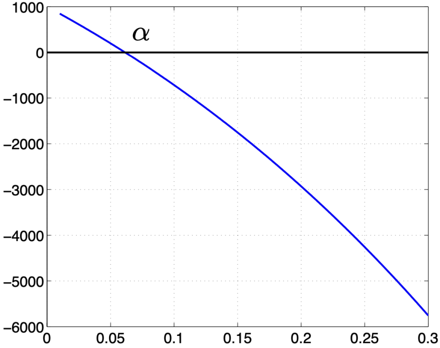
# Example 1 (Interest rates)

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));
```



# Example 1 (Interest rates)

- The root of $f$ is between 0.05 and 0.1.
- 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 $x = 0.061407470703125$.
- 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%.

# Examples of nonlinear equations

**Example 2 (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 $p$, $V$, and $T$) is:

$$\left(p + \frac{aN^2}{V^2}\right)(V - Nb) = kNT,$$

where $a$ and $b$ are two coefficients that depend on the specific gas, $N$ is the number of molecules contained in the volume $V$, and $k$ is the Boltzmann constant.

We consider the carbon dioxide ($CO_2$), for which $a = 0.401\,\text{Pa} \cdot \text{m}^6$ and $b = 42.7 \times 10^{-6}\,\text{m}^3$.
We search the volume occupied by $N = 1000$ molecules of $CO_2$ at temperature $T = 300\,\text{K}$ and pressure $p = 3.5 \times 10^7\,\text{Pa}$.

We know that the Boltzmann constant is $k = 1.3806503 \times 10^{-23}\,\text{Joule} \cdot \text{K}^{-1}$.

# Example 2 (State equation of a gas)

We draw the graph of the function

$$f(V) = \left(p + \frac{aN^2}{V^2}\right)(V - Nb) - kNT$$

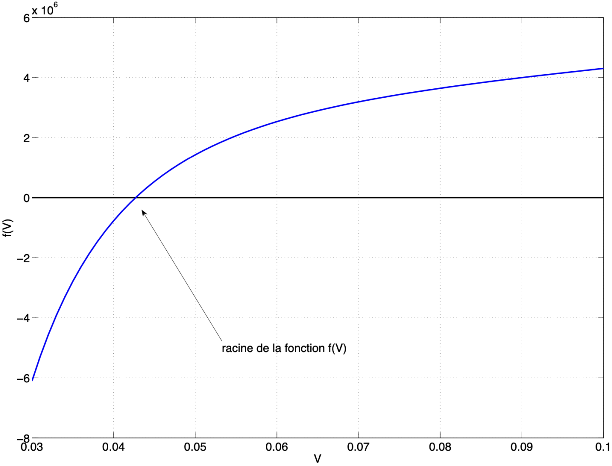
for $V > 0$. We do not consider $V < 0$ (it does not have physical sens), because V is the volume of gas.

We use the commands in Matlab:

```
>> 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
```

# Example 2 (State equation of a gas)

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



# Example 2 (State equation of a gas)

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 of $10^{-12}$:

$$[\text{zero}, \text{res}, \text{niter}] = \text{bisection}(f, 0.03, 0.1, 1 \times 10^{-12}, 1000, p, T, a, b, N, k);$$

then we find, after 36 iterations, the value $V = 0.0427$.
If we use the Newton method with the same tolerance, starting from 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 $0.0427\,\text{m}^3$.

# Modified Newton method

For the iterate of the modified Newton method

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

associate the iteration function $\phi_{mN}(x)$ defined as:

$$\phi_{mN}(x) = x - m\frac{f(x)}{f'(x)},$$

where $m$ is the multiplicity of the zero $\alpha$.

# Convergence of modified Newton

## Proposition 16 (Proposition 2.16 from book)

*If $f \in C^m(I_\alpha)$, with $I_\alpha$ a neighborhood of the zero $\alpha$ and $m-1$ the multiplicity of $\alpha$, for the iteration function $\phi_{mN}(x)$, we have*

$$\phi'_{mN}(\alpha) = 1 - \frac{m}{m} = 0 \text{ for all } m \geq 1.$$

## Proof.

*The result follows analogously to that of Proposition 2.13, reported in exercise series* □

## Corollary 17 (Corollary 2.17 from book)

*If $f \in C^2(I_\alpha) \cap C^m(I_\alpha)$, $\alpha$ is a zero of multiplicity $m-1$, and $x^{(0)}$ is "sufficiently" close to $\alpha$, then the modified Newton method converges with order 2 (quadratically).*

## Proof.

*From Proposition 2.11, 2.12, 2.16.* □

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