Numerical methods

Solving nonlinear equations

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton’s (Newton-Raphson) method
8. Steffensen’s method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Solving nonlinear equation

$$f(x)=0 \tag{1}$$

means to find such points $x^* \in \Re$ that

$$f(x^*)=0.$$

We call such point **roots of function** $f(x)$.

In general, we do not know (because it is impossible) the explicit formula for roots of $f(x)$.

Iterative methods:

we generate sequence of approximations

$$x_0, x_1, x_2, \ldots$$

from one or several initial approximations (guess) of root x^*,

which converge to the root x^*.

Introduction

For some methods it is enough
to prescribe interval $\langle a,b \rangle$,
which contains the searched root,
other require
initial guess to be
reasonably close to the true root.

Usually we start with robust
but reliable method
and then,
when we are close enough to the root,
we switch to more sophisticated
and faster convergent method.

Introduction

For simplicity, we will consider only problem of finding
simple root x^* of function $f(x)$,
i.e. we suppose that $f'(x^*) \neq 0$.

We will also suppose that
function $f(x)$ is continuous and
has so many continuous derivatives,
how many we need.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton's (Newton-Raphson) method
8. Steffensen's method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Root separation and estimation of initial approximation

In order to find solutions of

$$f(x)=0$$

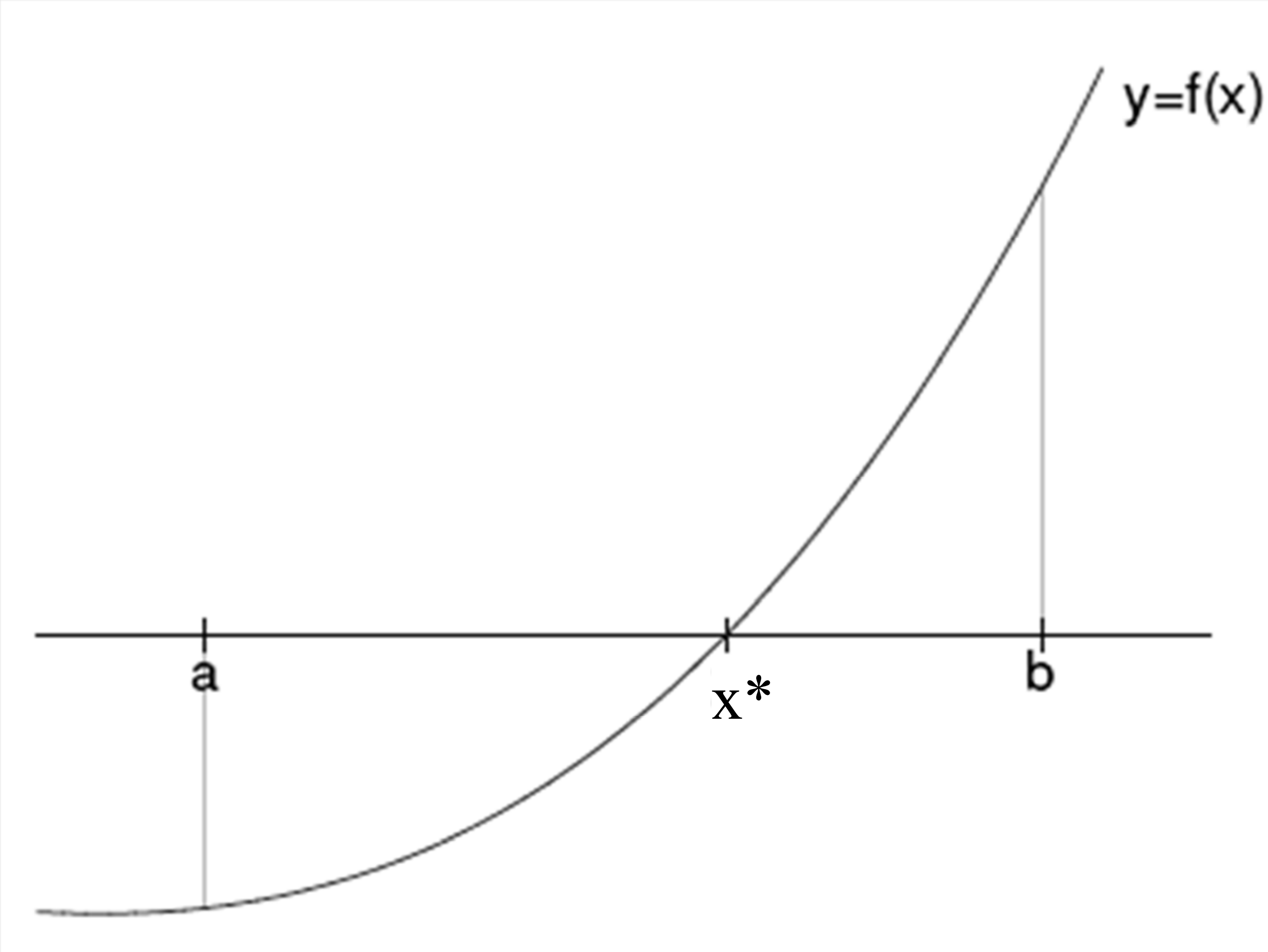
we have to estimate
the number of roots
and
we have to determine intervals
containing a unique root.

Theorem: If the function is continuous on interval $\langle a,b \rangle$ and

$$f(a)\cdot f(b)<0,$$

then there is at least one root of $f(x)=0$ on interval $\langle a,b \rangle$.

Root separation and estimation of initial approximation



Root separation and estimation of initial approximation

We can find the initial approximation of roots of

$$f(x)=0$$

from graph of function $f(x)$.

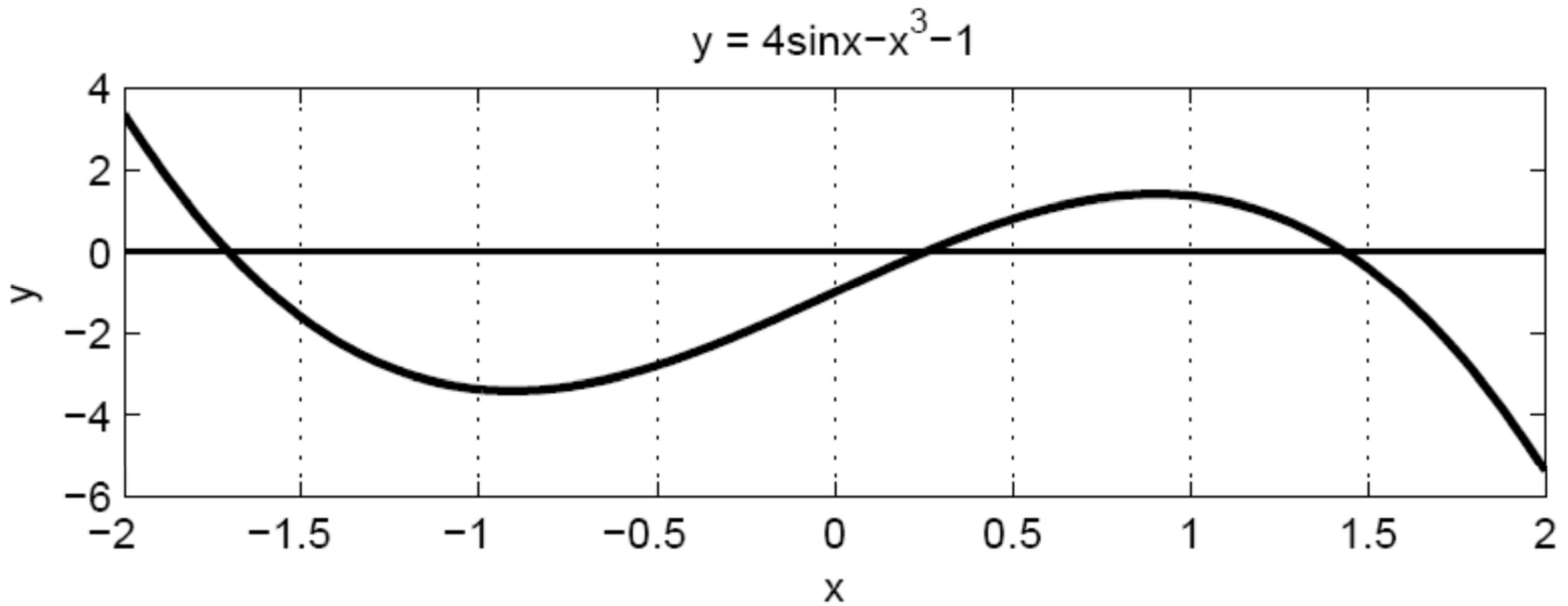
Other possibility is to assemble the table of points $\left[x_i, f\left(x_i\right)\right]$ for some division

$$a = x_0 < x_1 < \cdots < x_{i-1} < x_i < \cdots < x_n = b$$

of chosen interval $\langle a,b \rangle$.

Example: Obtain rough guess of roots of equation $f(x)=0$, where

$$f(x) = 4\sin x - x^3 - 1.$$

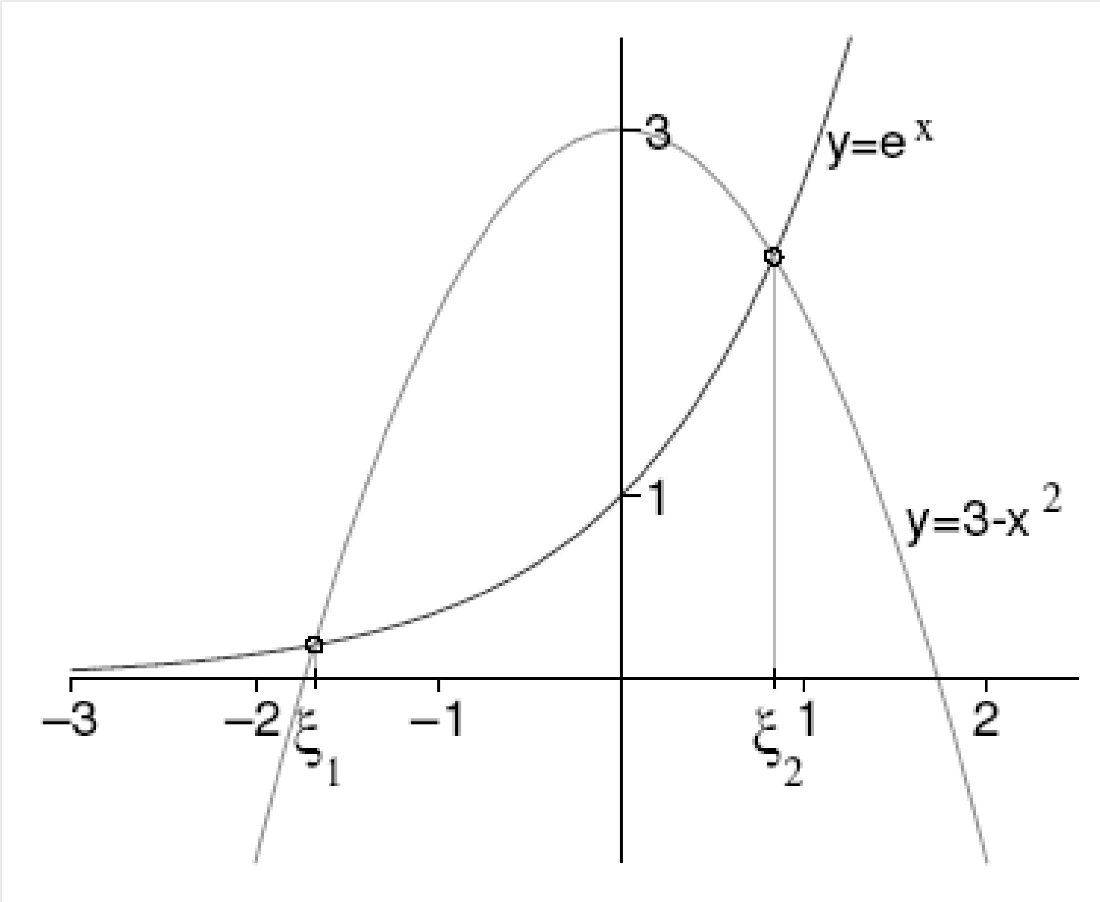


Example: Obtain a rough guess of roots of equation

$$e^x + x^2 - 3 = 0$$

Solution: Rearrange the equation as follows

$$e^x = 3 - x^2$$



CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. **Bisection method**
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton's (Newton-Raphson) method
8. Steffensen's method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

It is based on the principle of sign changes.

Let suppose that function values of $f(a_0)$ and $f(b_0)$ at endpoints of interval (a_0, b_0) are of opposite signs,

i.e. $f(a_0)\cdot f(b_0) < 0$.

We will construct a sequence of intervals

$$(a_0, b_0) \supset (a_1, b_1) \supset (a_2, b_2) \supset (a_3, b_3) \supset \cdots,$$

containing the root.

Intervals $(a_{k+1}, b_{k+1}),\ k = 0, 1, \ldots$ are determined recursively as follows:

Bisection method

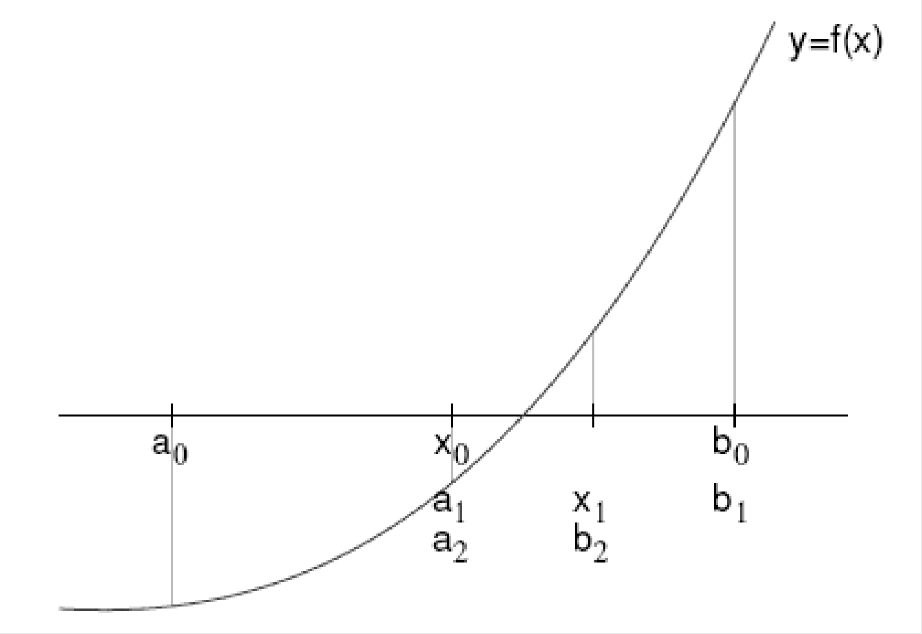
Find a midpoint of interval (a_k, b_k) and designate it $x_{k+1} = \frac{1}{2}(a_k + b_k)$.

If $f(x_{k+1}) = 0$ then $x^* = x_{k+1}$ and stop.

If $f(x_{k+1}) \neq 0$ then

$$(a_{k+1}, b_{k+1}) = \begin{cases} (a_k, x_{k+1}), & \text{if} \quad f(a_k) f(x_{k+1}) < 0, \\ (x_{k+1}, b_k), & \text{if} \quad f(a_k) f(x_{k+1}) > 0. \end{cases}$$

From construction of (a_{k+1}, b_{k+1}) it follows that $f(a_{k+1}) f(b_{k+1}) < 0$, so each interval (a_k, b_k) contains a root.



Bisection method

After k steps the root is in interval $I_k := (a_k, b_k)$ with length

$$\left|I_k\right| = b_k - a_k = \frac{b_{k-1} - a_{k-1}}{2} = \cdots = 2^{-k}\left(b_0 - a_0\right).$$

Midpoint x_{k+1} of interval $\left(a_k, b_k\right)$ is an approximation of x^* with an error

$$\left|x_{k+1} - x^*\right| \le \tfrac{1}{2}\left(b_k - a_k\right) = 2^{-k-1}\left(b_0 - a_0\right). \qquad (2)$$

For $k \to \infty$ obviously $\left|I_k\right| \to 0$ and $x_k \to x^*$.

Example: How many iterations by bisection method we have to perform in order to refine the root by one decimal digit?

Bisection method

Bisection method converge slowly
but the convergence is always guaranteed.

The rate of convergence (2) does not depend on function $f(x)$,
because we used only signs of function values.

If we efficiently use those values
(and possibly also values of derivatives $f'(x)$),
we could achieve faster convergence.

Such "refined" methods usually converge
only if we starts from good initial approximation.
Most often such initial guess is obtained by bisection method.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton's (Newton-Raphson) method
8. Steffensen's method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Let $x_0, x_1, x_2, \ldots$ is a sequence which converges to x^* and $e_k = x_k - x^*$. If there exists number p and constant $C \neq 0$ such that

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^p} = C, \tag{3}$$

then p is called **the order of convergence** and
C is **error constant**.

We say that

	linear,		$p = 1$ and $C < 1$,
convergence is	superlinear,	if	$p > 1$,
	quadratic,		$p = 2$.

Rate of convergence

Let $x_0, x_1, x_2, \ldots$ is a sequence which converges to x^* and $e_k = x_k - x^*$. If there exists number p and constant $C \neq 0$ such that

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^p} = C, \tag{3}$$

then p is called **the order of convergence** and
C is **error constant**.

We say that

$$\text{convergence is} \quad \begin{array}{l} \text{linear,} \\ \text{superlinear,} \\ \text{quadratic,} \end{array} \quad \text{if} \quad \begin{array}{l} p = 1 \quad \text{and} \quad C < 1, \\ p > 1, \\ p = 2. \end{array}$$

We say that the **method converges with order** p ,
if all convergent sequences obtained by this method
have the order of convergence greater or equal to p and
at least one of them has order of convergence exactly equal to p.

Example: What is the order of convergence of bisection method?

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^p} = C, \qquad e_k = x_k - x^*$$

Example: What is the order of convergence of bisection method?

Midpoint x_{k+1} of interval (a_k, b_k) is an approximation of x^* with error

$$\left|x_{k+1} - x^*\right| \le \tfrac{1}{2}\left(b_k - a_k\right) = 2^{-k-1}\left(b_0 - a_0\right).$$

$$\lim_{k\to\infty} \frac{\left|x_{k+1} - x^*\right|}{\left|x_k - x^*\right|^p} = \frac{2^{-k-1}\left(b_0 - a_0\right)}{\left[2^{-k}\left(b_0 - a_0\right)\right]^p} = \frac{1}{2}\left(\frac{2^k}{b_0 - a_0}\right)^{p-1}$$

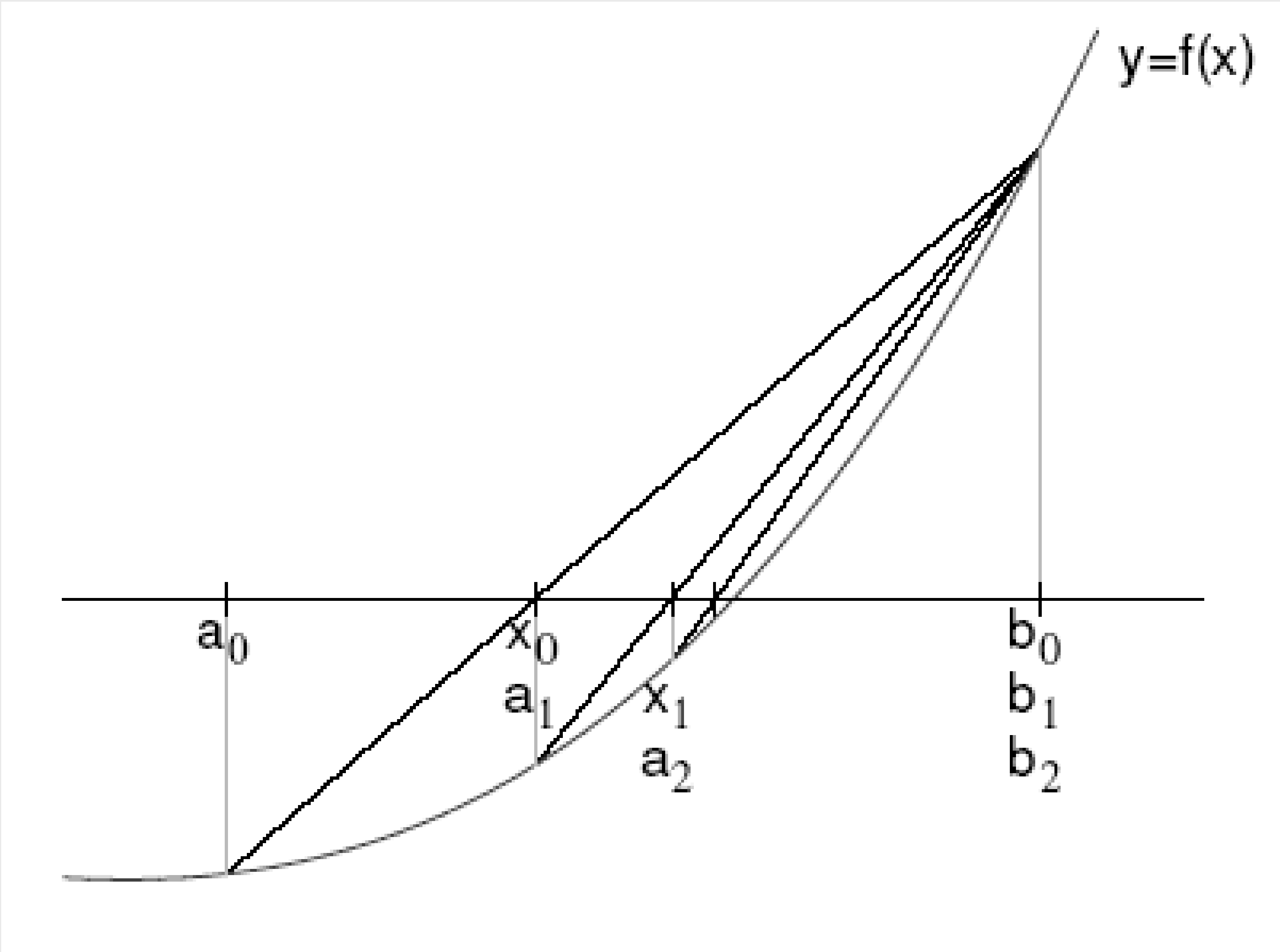
$$p = 1, \quad C = \frac{1}{2}$$

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton's (Newton-Raphson) method
8. Steffensen's method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Regula falsi (false position) method

It is very similar to bisection method.
However, the next iteration point is not midpoint of interval
but intersection of axis x with secant through $[a_k, f(a_k)]$ and $[b_k, f(b_k)]$.



Regula falsi (false position) method

The root of secant we estimate by

$$x_{k+1} = b_k - \frac{b_k - a_k}{f(b_k) - f(a_k)} f(b_k)$$

If $f(x_{k+1}) = 0$ then $x^* = x_{k+1}$ and stop.
If $f(x_{k+1}) \neq 0$ then

$$(a_{k+1}, b_{k+1}) = \begin{cases} (a_k, x_{k+1}), & \text{if} \quad f(a_k) f(x_{k+1}) < 0, \\ (x_{k+1}, b_k), & \text{if} \quad f(a_k) f(x_{k+1}) > 0. \end{cases}$$

From construction of (a_{k+1}, b_{k+1}) it follows that $f(a_{k+1}) f(b_{k+1}) < 0$,
so each interval (a_k, b_k) contains a root.

Regula falsi (false position) method

After k steps the root is in interval $I_k := (a_k, b_k)$.

Unlike the bisection method the length of interval $|I_k|$ in some cases **fail to converge** to a zero limit.

Regula falsi method always converges.

The rate of convergence is
(similarly as bisection method)
linear.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton's (Newton-Raphson) method
8. Steffensen's method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Secant method

It is similar to regula falsi method.

We start from interval $\langle a,b \rangle$ containing the root.

Denote $x_0 = a$ and $x_1 = b$.

Let secant goes through points $[x_0, f(x_0)]$ and $[x_1, f(x_1)]$ and
its intersect with axis x
we denote x_2 .

Unlike the regula falsi method
we will not select an interval containing the root but
we construct secant through points $[x_1, f(x_1)], [x_2, f(x_2)]$,
and its root we denote x_3.

Secant method

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We start from interval $\langle a,b\rangle$ containing the root.

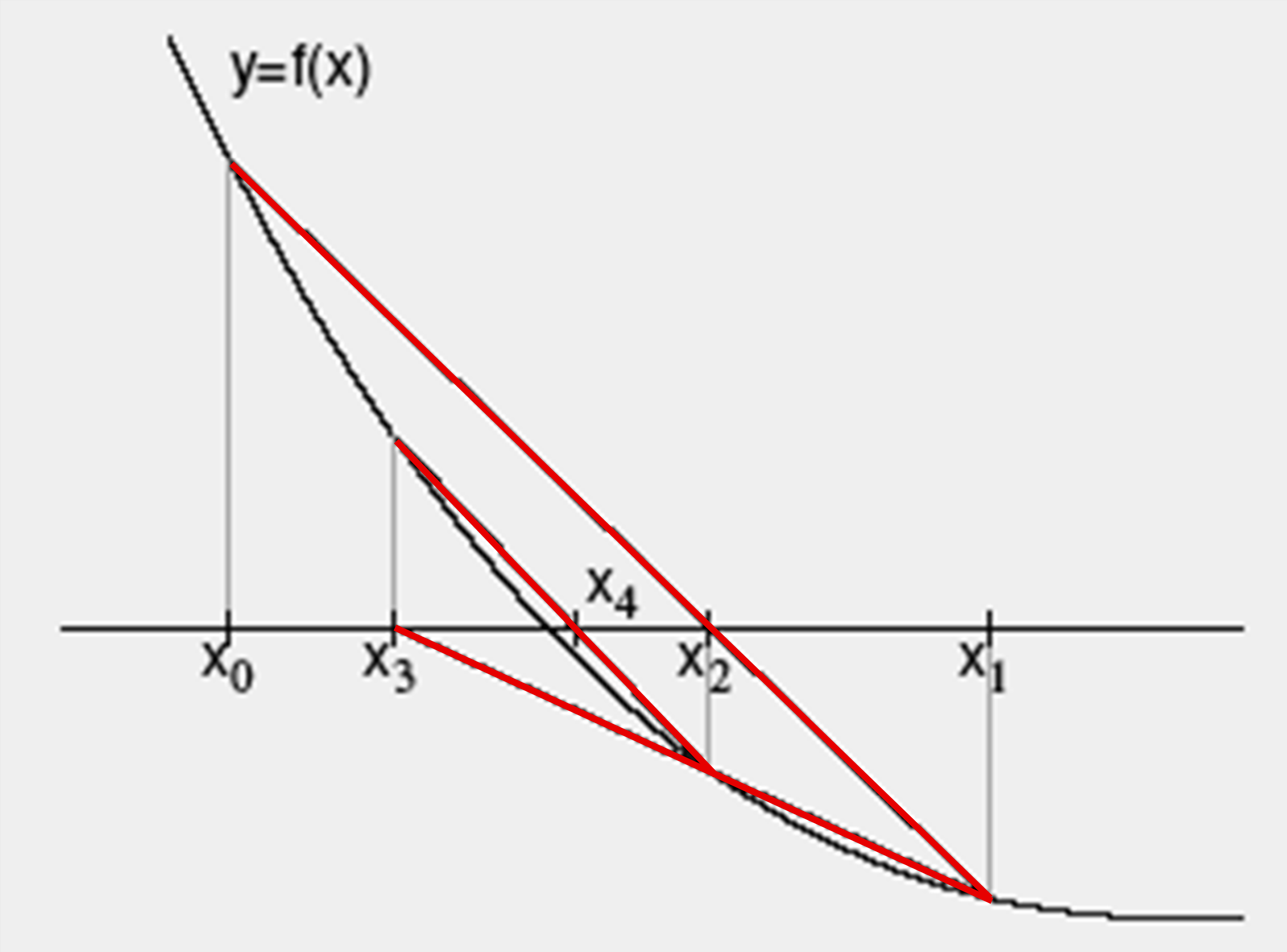
Denote $x_0 = a$ and $x_1 = b$.

Let secant goes through points $[x_0, f(x_0)]$ and $[x_1, f(x_1)]$ and
its intersect with axis x
we denote x_2 .

Unlike the regula falsi method
we will not select an interval containing the root but
we construct secant through points $[x_1, f(x_1)], [x_2, f(x_2)]$,
and its root we denote x_3.

Then we construct secant through $[x_2, f(x_2)]$ and $[x_3, f(x_3)]$ and so on.

Secant method



Secant method

The k-th approximation of root is obtained by

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f\left(x_k\right) - f\left(x_{k-1}\right)} f\left(x_k\right),$$

where $x_0 = a,\ x_1 = b.$

The computation is finished if **stop criterion** is hold.

$$\left|x_{k+1} - x_k\right| \le \varepsilon, \qquad \text{or} \qquad \left|x_{k+1} - x_k\right| \le \varepsilon \left|x_k\right|,$$

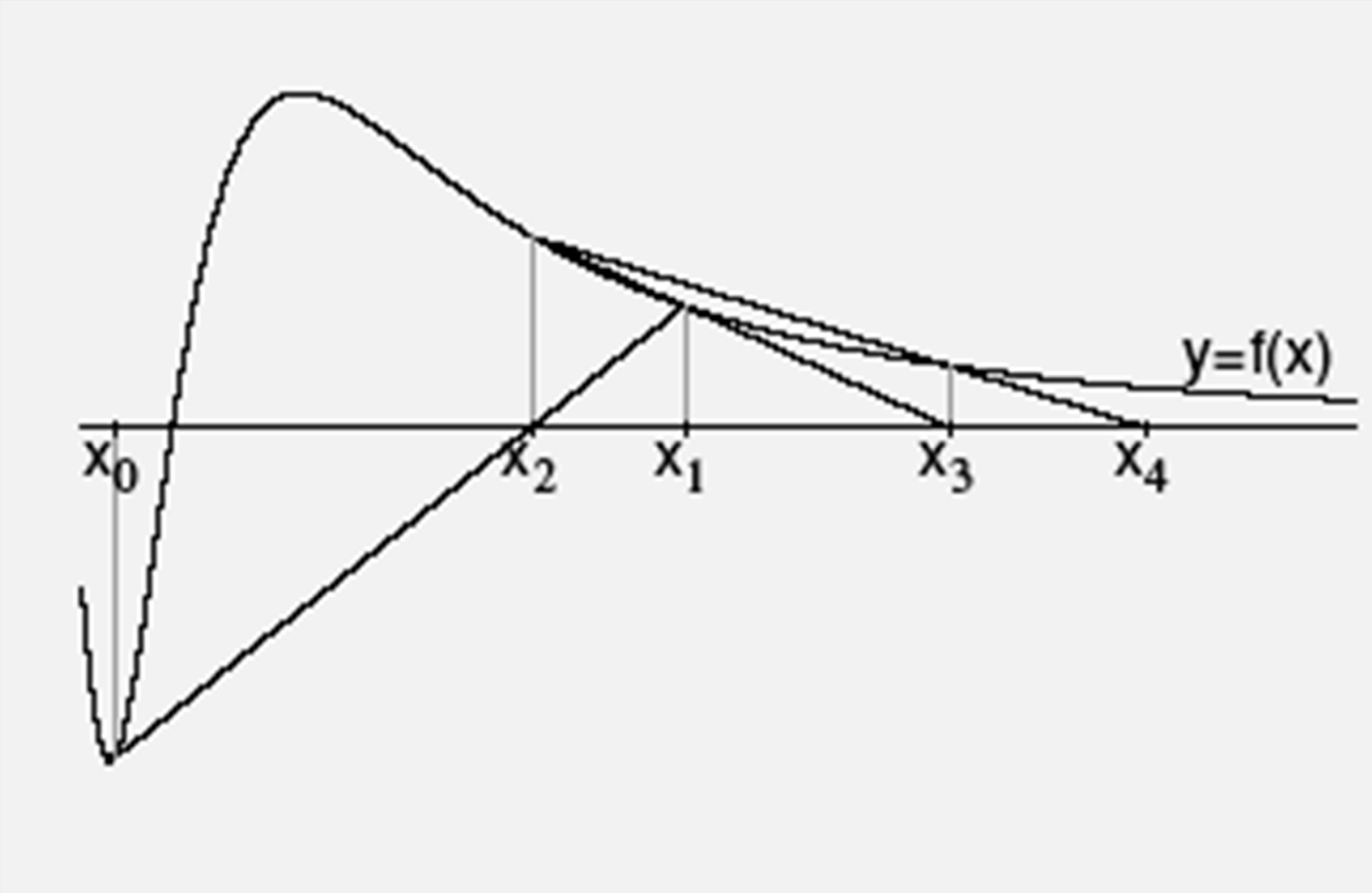
$$\text{or} \qquad \left| f\left(x_{k+1}\right) \le \varepsilon, \right|$$

or if we find the root.

Caution! The condition does not guarantee that $\left|x_{k+1} - x^*\right| \le \varepsilon.$

Example: How we can check the condition $\left|x_{k+1} - x^*\right| \le \varepsilon$?

Secant method could be divergent !



Secant method

Secant method converge faster than regula falsi,
but could also diverge.

It converge
if initial points x_1 and x_2 are close enough to root x^*.

Is it possible to show, that convergence rate is

$$p = \frac{1}{2}\left(1+\sqrt{5}\right) \doteq 1.618\,,$$

i.e. the secant method is **superlinear**.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton's (Newton-Raphson) method
8. Steffensen's method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

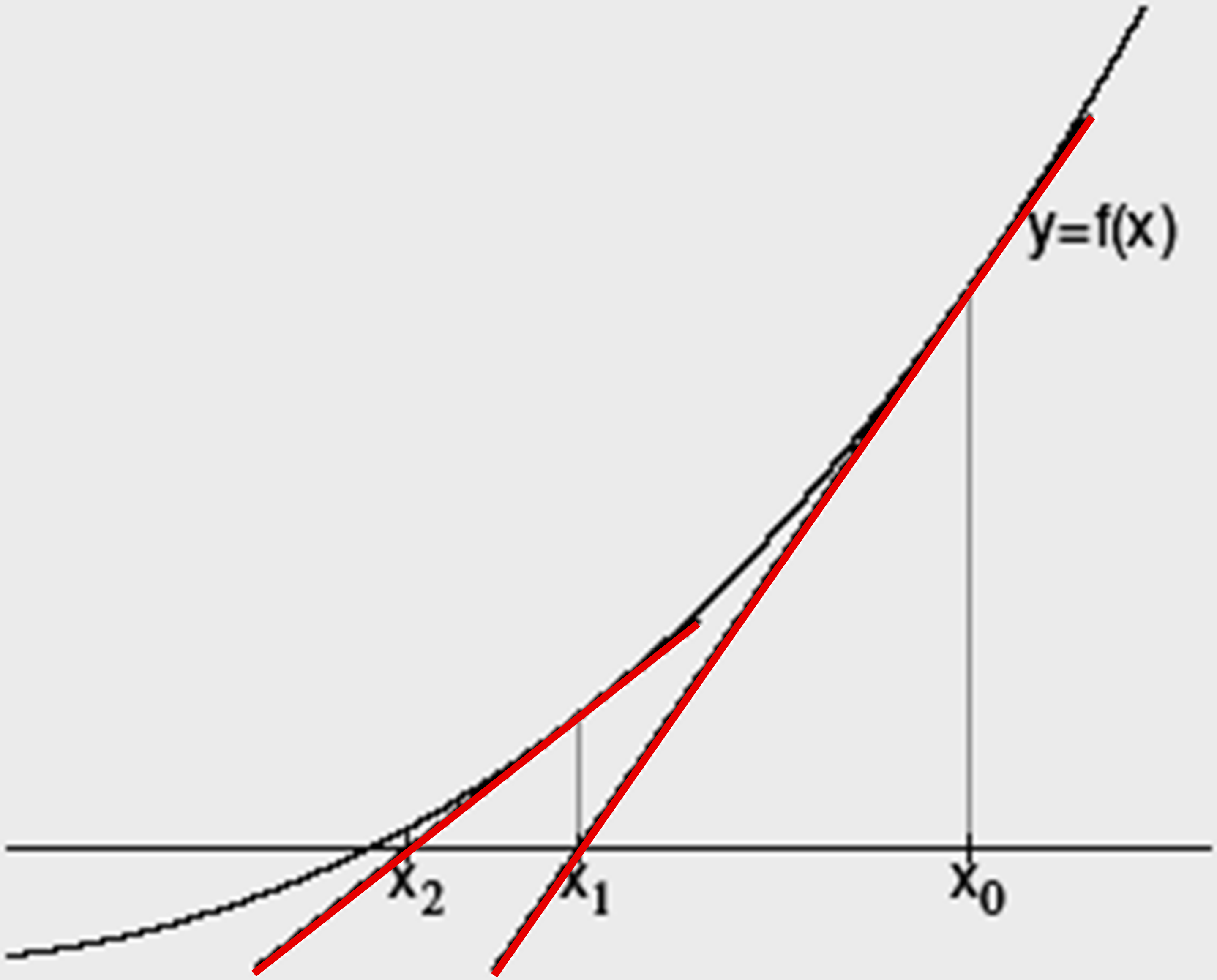
Newton's (Newton-Raphson) method

We will work with tangent
of the graph of function f.

Therefore we suppose that f is differentiable.

We chose the initial approximation of the root x_0.
We route a tangent line
to the graph of function f through point $\left[x_0, f\left(x_0\right)\right]$.
The intersect with axis x will be x_1.
Then we route a tangent line through $\left[x_1, f\left(x_1\right)\right]$,
The intersect with axis x will be x_2 ,
and so on.

Newton's (Newton-Raphson) method



Newton's (Newton-Raphson) method

Suppose that we know x_k

and we want to find better approximation x_{k+1}.

We construct the tangent line to the curve $y = f(x)$ through $[x_k, f(x_k)]$.

Using equation for the tangent line

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

with $y := 0$ we obtain an intersect with the axis x :

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} .$$

Newton's (Newton-Raphson) method - convergence

Let $e_k = x_k - x^*$ be an error in the k-th step.

Lets construct the Taylor expansion of $f(x^*)$ at x_k

$$0 = f(x^*) = f(x_k) + (x^* - x_k) f'(x_k) + \frac{1}{2}(x^* - x_k)^2 f''(\xi),$$

where ξ is some point of interval with endpoints x_k and x^*.

After some algebra we obtain

$$-\frac{1}{2}(x^* - x_k)^2 \frac{f''(\xi)}{f'(x_k)} = \frac{f(x_k)}{f'(x_k)} + (x^* - x_k)$$

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After some algebra we obtain

$$-\frac{1}{2}(x^* - x_k)^2 \frac{f''(\xi)}{f'(x_k)} = \frac{f(x_k)}{f'(x_k)} + (x^* - x_k)$$

$$-\frac{1}{2}(x^* - x_k)^2 \frac{f''(\xi)}{f'(x_k)} = x^* - \left[x_k - \frac{f(x_k)}{f'(x_k)} \right]$$

Newton's (Newton-Raphson) method - convergence

Let $e_k = x_k - x^*$ be an error in the k-th step.

Lets construct the Taylor expansion of $f(x^*)$ at x_k

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After some algebra we obtain

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Let $e_k = x_k - x^*$ be an error in the k-th step.

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$$0 = f(x^*) = f(x_k) + (x^* - x_k) f'(x_k) + \frac{1}{2}(x^* - x_k)^2 f''(\xi),$$

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After some algebra we obtain

$$-\frac{1}{2}(x^* - x_k)^2 \frac{f''(\xi)}{f'(x_k)} = \frac{f(x_k)}{f'(x_k)} + (x^* - x_k)$$

$$-\frac{1}{2}(x^* - x_k)^2 \frac{f''(\xi)}{f'(x_k)} = x^* - \left[x_k - \frac{f(x_k)}{f'(x_k)}\right] = x^* - x_{k+1}$$

$$\frac{1}{2} \quad e_k^{\ 2} \qquad \frac{f''(\xi)}{f'(x_k)} = e_{k+1}$$

Newton's (Newton-Raphson) method - convergence

$$\frac{1}{2}{e_k}^2 \frac{f''(\xi)}{f'(x_k)} = e_{k+1} \tag{4}$$

After applying a limit

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^2} = 2\frac{|f''(\xi)|}{|f'(x_k)|}.$$

Recall the definition of the rate of convergence:

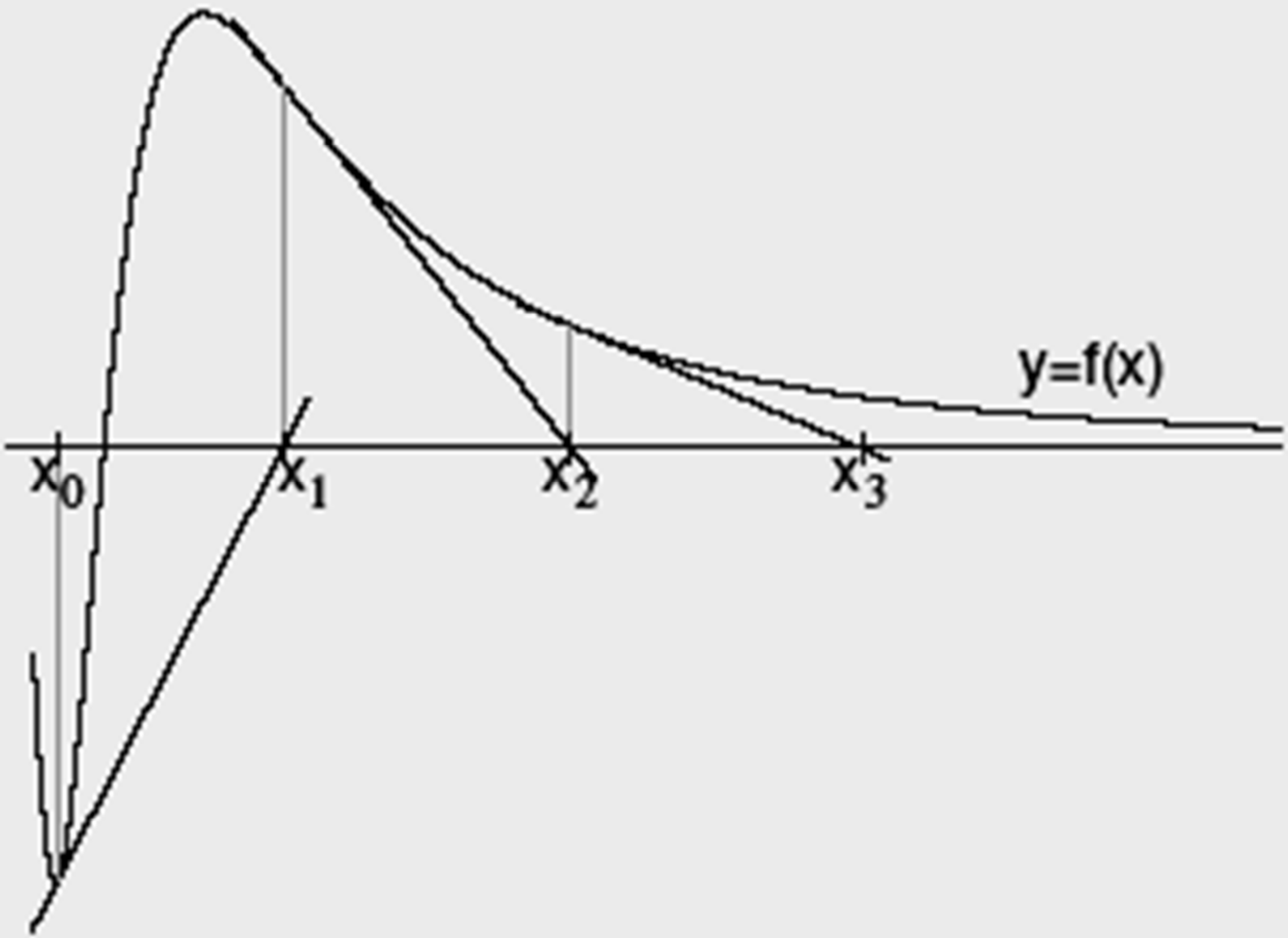
Let $x_0, x_1, x_2, \ldots$ is a sequence which converges to x^* and $e_k = x_k - x^*$. If there exists number p and constant $C \neq 0$ such that

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^p} = C,$$

then p is called **the order of convergence** and C is **error constant**.

Newton's method converges **quadratically**.

Newton's (Newton-Raphson) method - convergence



Newton's method can also diverge

Newton's (Newton-Raphson) method - convergence

Question: After which condition the is the Newton's method convergent?

Suppose that in some vicinity I of the root it holds

$$\frac{1}{2}\frac{f''(y)}{f'(x)} \le m \qquad \text{for all} \qquad x \in I, \; y \in I.$$

If $x_k \in I$, then from (4) follows

$$|e_{k+1}| \le m|e_k|^2 \qquad \text{or} \qquad |me_{k+1}| \le |me_k|^2 \; .$$

Repeating this idea we get

$$|me_{k+1}| \le |me_k|^2 \le |me_{k-1}|^4 \le |me_{k-2}|^8 \le \cdots \le |me_0|^{2k+1}$$

If $|me_0| < 1$, then for sure $|e_{k+1}| \to 0$ and therefore $x_{k+1} \to x^*$.

Newton's method is always convergent
if the initial approximation is sufficiently close to the root.

Combined method

Good initial approximation x_0 can be obtained by bisection method.

Combination of bisection and Newton's method leads to
a **combined method**,
which is always convergent.

e.g. procedure **`rtsafe`** from Numerical Recipes;
Newton's method is applied only in the vicinity of the root,
otherwise the bisection method is used.
This assures the fast convergence.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton’s (Newton-Raphson) method
8. Steffensen’s method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Steffensen's method

Steffensen's method is modified Newton's method

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \;,$$

where the derivative f' is approximated by

$$f'(x) \approx \frac{f(x_k + h_k) - f(x_k)}{h_k} \;,$$

and h_k is number, which tends to zero for greater k.

We chose $h_k = f(x_k)$.

Unlike the secant method we have one more function evaluation.
However, is it possible to show that
the rate of convergence is the same
as in Newton's method, i.e., quadratic.

CONTENTS

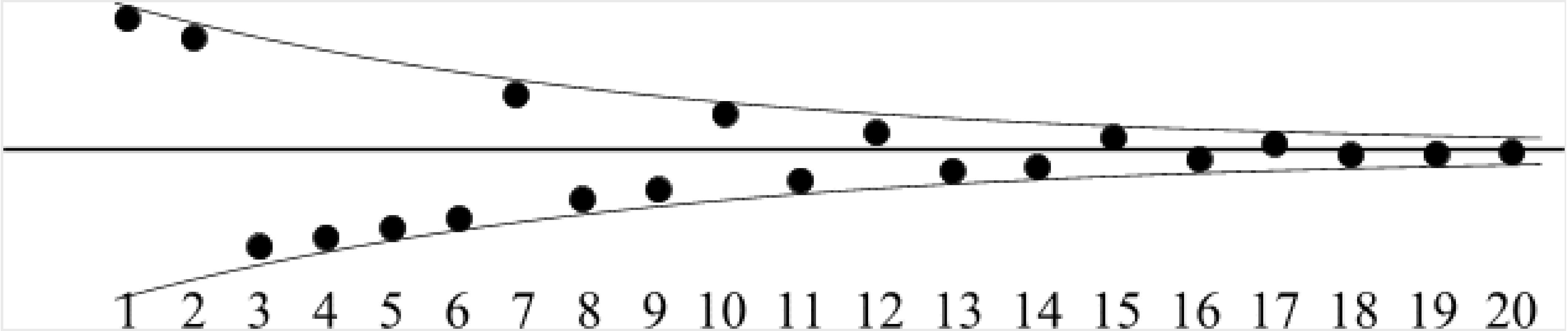
1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton’s (Newton-Raphson) method
8. Steffensen’s method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Metric space

A **metric space** is an ordered pair (X, d) where X is a set and d is a metric on X, such that for any $x, y, z \in X$, the following holds:

1. $d(x,y) \geq 0$
2. $d(x,y) = 0 \Leftrightarrow x = y$
3. $d(x,y) = d(y,x)$
4. $d(x,z) \leq d(x,y) + d(y,z)$

Convergence: If there is some distance ε such that no matter how far you go out in the sequence, you can find all subsequent elements which are closer to the limit than ε

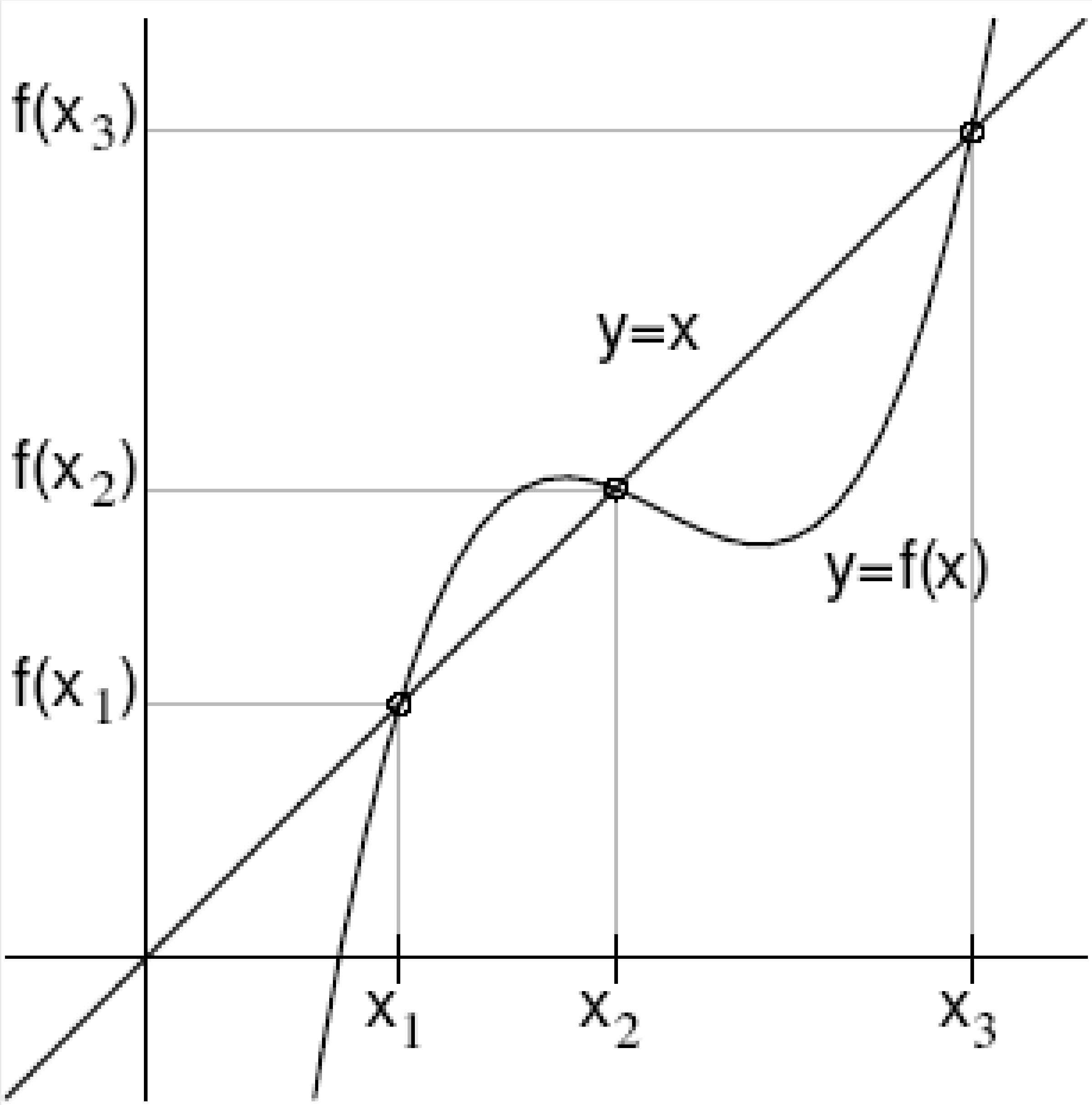


Cauchy sequence <- term in functional analysis

Definition: Metric space is **complete** if
each Cauchy sequence has limit in the space

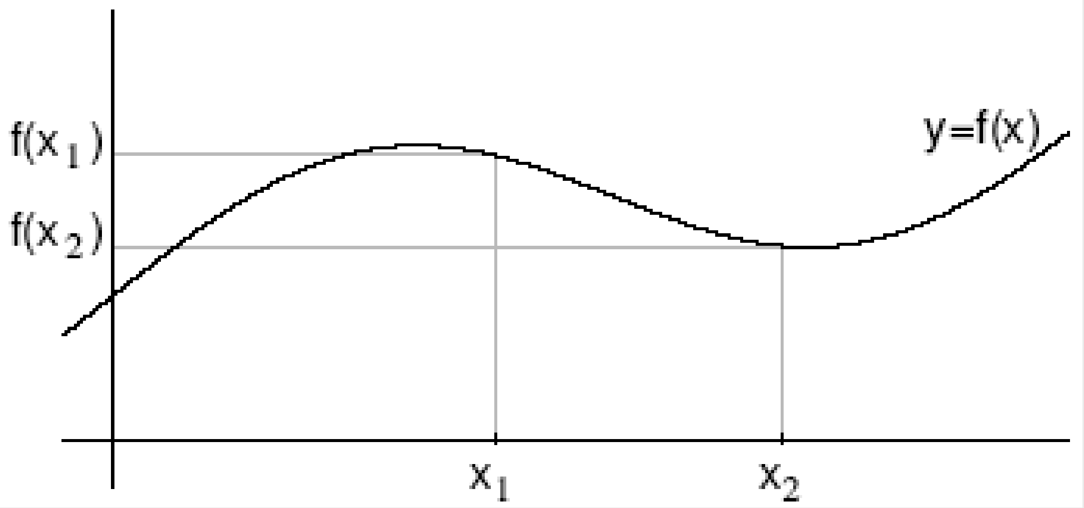
Definition: The element $x \in X$ is called **fixed point**
of mapping $F : X \to X$,
if $F(x) = x$.

Functional analysis



Contraction mapping: images of two elements are closer then originals

$$\forall x, y \in M \quad d\left(F\left(x\right), F\left(y\right)\right) \leq \alpha d\left(x, y\right); \quad \alpha \in \left\langle 0,1\right)$$



Banach fixed-point theorem:

Let (X, d) be a non-empty complete metric space with a contraction mapping $g : X \longrightarrow X$. Then g admits a unique fixed-point x^* in X. Furthermore, x^* can be found as follows:

start with an arbitrary element x_0 in X and define a sequence $\{x_n\}$ by $g(x_{n-1}) = x_n$, then $x_n \longrightarrow x^*$.

Fixed-point iteration

What it is good for? Suppose we want to solve $f(x)=0$.

Let's rewrite the $f(x)=0$ as $\underbrace{\frac{f(x)}{h(x)}+x}_{g(x)}=x$, assuming $h(x)\neq 0$

We'll get fixed-point problem for $g(x)$

while the solution of $g(x_p)=x_p$

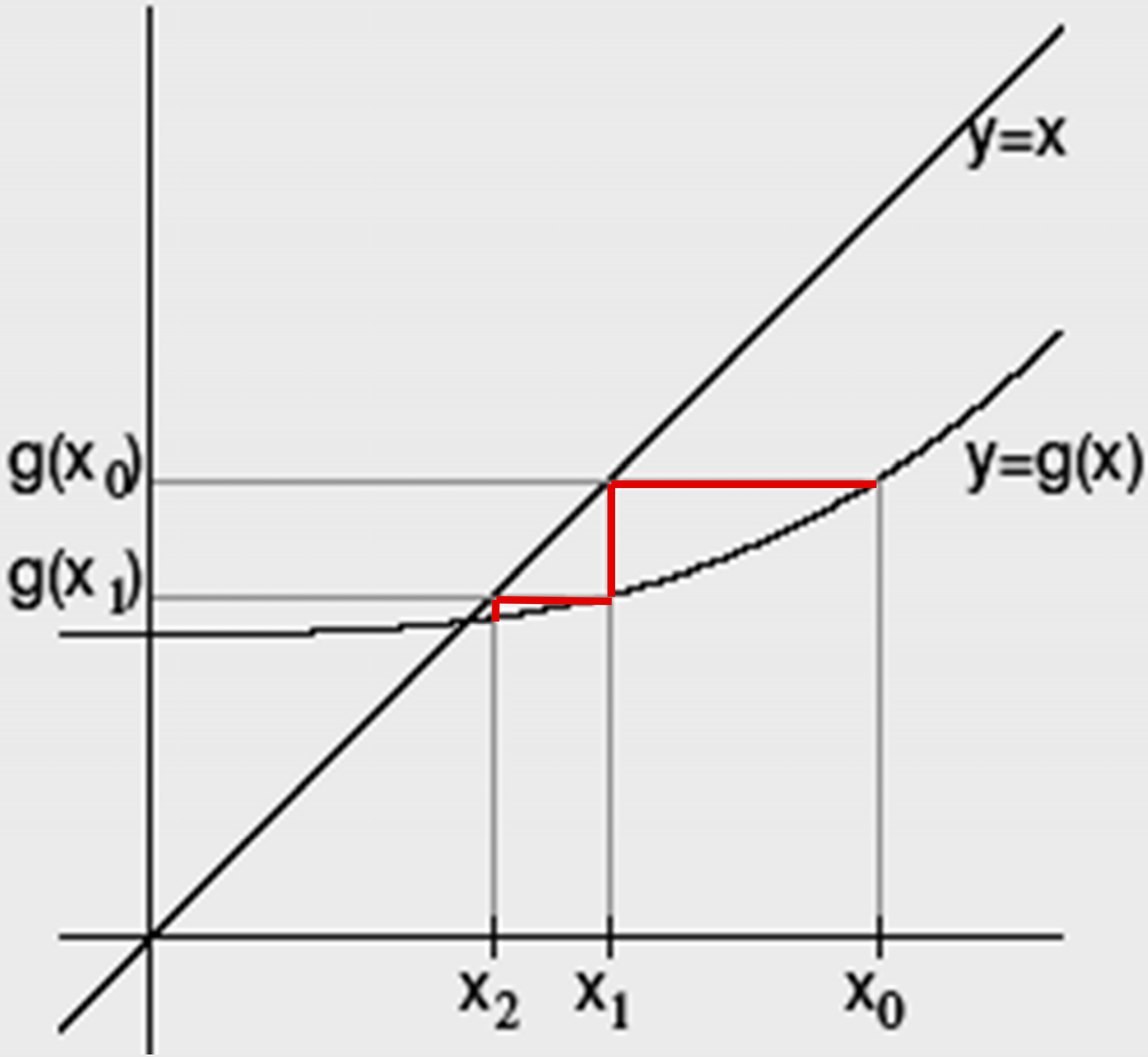
is root of $f(x_p)=0$.

Function g is called the **iterative** function.

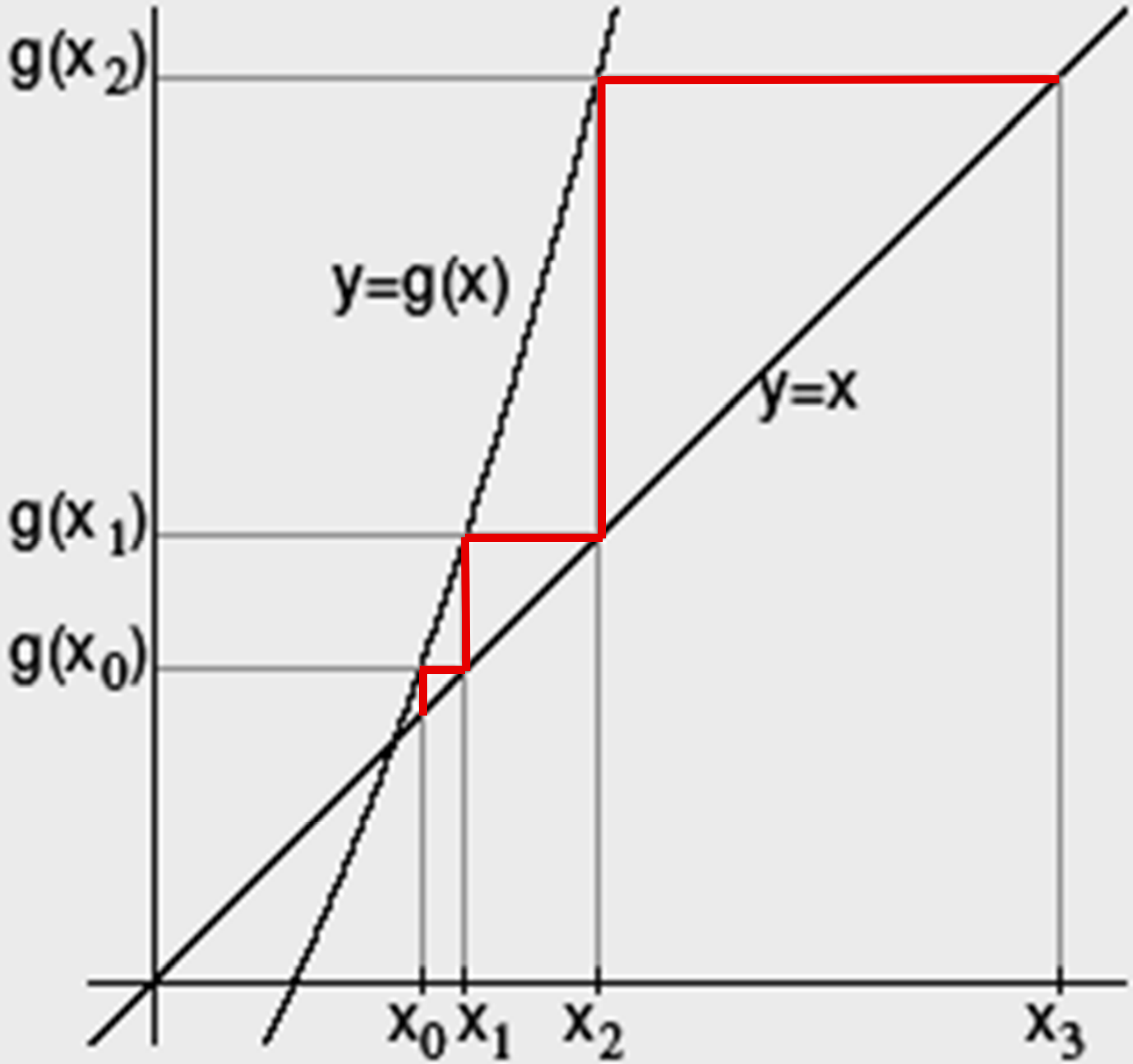
We will chose the initial approximation x_0 and

next iterations will be $x_{k+1}=g\left(x_k\right)$.

Fixed-point iteration



This way not always leads to the fixed point of g.



Fixed-point iteration

We said that
fixed-point iteration method converges
if the iterative function is
contraction mapping.

In case of function of one variable,
contraction closely relates to
the rate of increase of function.

Theorem:

Let function g maps an interval $\langle a,b\rangle$ to itself

and g is derivative on this interval.

If there exists number $\alpha \in \langle 0,1)$ so that

$$\left|g'(x)\right| \le \alpha \quad \forall x \in \langle a,b\rangle \ ,$$

then there exists fixed point x^* of function g in interval $\langle a,b\rangle$ and sequence of iterations

$$x_{k+1} = g\left(x_k\right)$$

converges to the fixed point for any initial approximation $x_0 \in \langle a,b\rangle$.

Next it holds

$$\left|x_k - x^*\right| \le \frac{\alpha}{1-\alpha}\left|x_k - x_{k-1}\right|.$$

Then is it possible to show, that convergence is linear.

Fixed-point iteration

The are many ways how to express x from the $f(x)=0$.

One possibility is to divide the equation $f(x)=0$ by its derivative f',
then multiply the equation by -1
and after all we add to both sides of equation x.
We get

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

Newton's method is a special case
of fixed-point iteration method.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton’s (Newton-Raphson) method
8. Steffensen’s method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Aitken Extrapolation

Recall the definition of the rate of convergence:

Let $x_0, x_1, x_2, \ldots$ is a sequence which converges to x^* and $e_k = x_k - x^*$. If there exists number p and constant $C \neq 0$ such that

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^p} = C,$$

then p is called **the order of convergence** and C is **error constant**.

Suppose the linear convergence of an iterative method

$$x_{k+1} = g(x_k),$$

i.e. it holds

$$\lim_{k\to\infty} \frac{|x_k - x^*|}{|x_{k-1} - x^*|} \leq C.$$

Aitken Extrapolation

We can speed-up the convergence of fixed-point iteration as follows:
Suppose that $k \gg 1$. Then it approximately holds

$$x_k \quad - x^* \approx C\left(x_{k-1} - x^*\right),$$

$$x_{k+1} - x^* \approx C\left(x_k \quad - x^*\right),$$

from which we could express the fixed point x^*

$$\frac{x_k - x^*}{x_{k+1} - x^*} \approx \frac{x_{k-1} - x^*}{x_k - x^*}$$

$$\left(x_k - x^*\right)^2 \approx \left(x_{k+1} - x^*\right)\left(x_{k-1} - x^*\right)$$

$$x_k^2 - 2x_k x^* + x^{*2} \approx x_{k+1}x_{k-1} - x^*\left(x_{k+1} + x_{k-1}\right) + x^{*2}$$

$$x_k^2 - x_{k+1}x_{k-1} \approx -x^*\left(x_{k+1} + x_{k-1} + 2x_k\right)$$

$$x^* \approx \frac{x_{k+1}x_{k-1} - x_k^2}{x_{k+1} + 2x_k + x_{k-1}}$$

Aitken Extrapolation

We can speed-up the convergence of fixed-point iteration as follows: Suppose that $k \gg 1$. Then it approximately holds

$$x_k - x^* \approx C\left(x_{k-1} - x^*\right),$$

$$x_{k+1} - x^* \approx C\left(x_k - x^*\right),$$

from which we could express the fixed point x^*

$$x^* \approx \frac{x_{k-1}x_{k+1} - x_k^2}{x_{k+1} - 2x_k + x_{k-1}} = x_{k-1} - \frac{\left(x_k - x_{k-1}\right)^2}{x_{k+1} - 2x_k + x_{k-1}},$$

where $x_k = g\left(x_{k-1}\right), \quad x_{k+1} = g\left(x_k\right) = g\left(g\left(x_{k-1}\right)\right).$

This way we can define the new iterative formula

$$x_{k+1} = x_k - \frac{\left(g\left(x_k\right) - x_k\right)^2}{g\left(g\left(x_k\right)\right) - 2g\left(x_k\right) + x_k}.$$

We obtained the **Aitken-Steffensen** iterative method for finding the fixed point x^* of function $g\left(x\right)$.

Aitken Extrapolation

If the initial approximation x_0
is close enough to fixed point x^* and
if $g'(x^*) \neq 1$,
then Aitken-Steffensen method converges quadratically.

If $g'(x^*) = 1$, The convergence of this method is slow.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton’s (Newton-Raphson) method
8. Steffensen’s method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

Note (About the multiplicity of roots)

We say that the root x^* of equation $f(x)=0$ has **multiplicity** $\boldsymbol{q}$,
if function $g(x)=f(x)/(x-x^*)^q$ is defined in point x^*
and there is a root of $f(x)$ in that point, i.e. if

$$0<|g(x^*)|<\infty\,.$$

If function $f(x)$ has a continuous derivatives up to order q
in the vicinity of the root x^* then

$$f^{(j)}(x^*)=0,\quad j=0,1,\ldots,q-1\,.$$

Some of before mentioned methods could be applied
for finding the multiple roots but the convergence is slower.

If we expect the multiple roots,
it is advisable to use the fact that
function $u(x)=f(x)/f'(x)$ has simple root.

A few notes

Note (On achievable accuracy)

Let x_k is an approximation of simple root of equation $f(x)=0$.
Using the mean value theorem we get

$$f(x_k)=f(x_k)-f(x^*)=f'(\xi)(x_k-x^*),$$

where ξ is some point between x_k and x^*.
Suppose that we work with approximate values

$$\tilde{f}(x_k)=f(x_k)+\delta_k,$$

Then the best

achievable accuracy of the root x^*

In that case $|f(x_k)|\le\delta$, so

$$|x_k-x^*|=\frac{|f(x_k)|}{|f'(x_k)|}\le\frac{\delta}{|f'(\xi)|}\approx\frac{\delta}{|f'(x^*)|}=:\varepsilon_x^*,$$

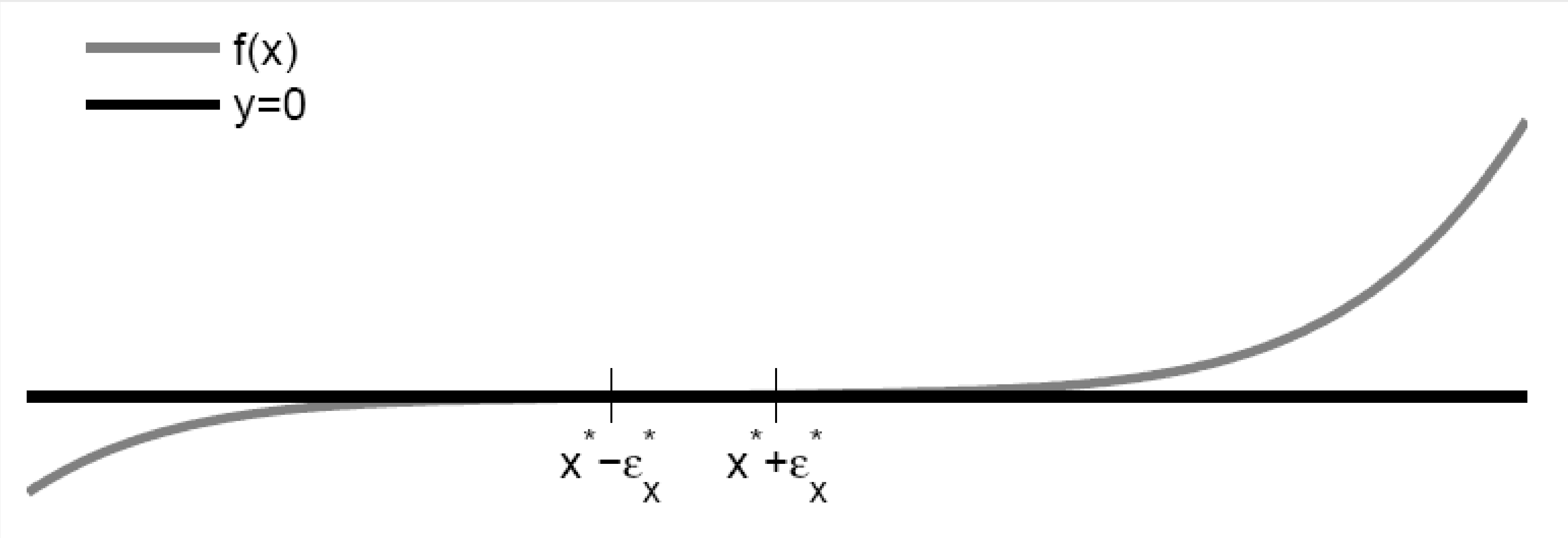
while f' is nearly constant in the vicinity of root.

It is impossible to compute x^* with error less than ε_x^*.

Note (On achievable accuracy)

If the slope $\left| f'\left(x^*\right) \right|$ in the root x^* is small,
then the achievable accuracy is large –

- **ill-conditioned problem**



Note (On achievable accuracy)

Similar consideration for the root of multiplicity q
imply the achievable accuracy

$$\varepsilon_x^* = \left(\frac{\delta \cdot q!}{f^{(q)}(x^*)} \right)^{1/q} .$$

The exponent $1/q$ causes that
the computation of multiple root
is in general ill-conditioned task.

CONTENTS

1. Introduction
2. Root separation and estimation of initial approximation
3. Bisection method
4. Rate of convergence
5. Regula falsi (false position) method
6. Secant method
7. Newton’s (Newton-Raphson) method
8. Steffensen’s method
9. Fixed-point iteration
10. Aitken Extrapolation
11. A few notes
12. Literature

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