MAT 460 Numerical Differential Equations

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Lecture 6

Topics: Nonlinear Equations and Iterative Methods in $\mathbb{R}$

Motivation: Many applications are nonlinear.

For example:

(1) Solve the equations

$$x = \cos(x), \qquad x = e^{-x}.$$

(2)
- Find the roots of a polynomial. Two examples: Solve

$$5x^7 - 3x^6 + x^3 - 1 = 0, \qquad x^2 - 5 = 0.$$

- Find all solutions to

$$\cos(x)\cosh(x) + 1 = 0.$$

Notation:

Problems of Type (1) are called **fix point problems**. We write in general

$$x = \phi(x)$$

with a given function $\phi(x)$.

Problems of Type (2) are called **root-finding problems** or factoring problems. We write in general

$$f(x) = 0$$

with a given function $f(x)$.

Fix point problems can be transformed into root-finding problems and conversely

Transforming a fix point problem $\rightsquigarrow$ a root-finding problem: Let

$$f(x) := x - \phi(x)$$

Then

$$x = \phi(x) \quad \Leftrightarrow \quad f(x) = 0.$$

Transforming a root-finding problem $\rightsquigarrow$ a fix point problem: Let

$$\phi(x) := x + a(x)\, f(x).$$

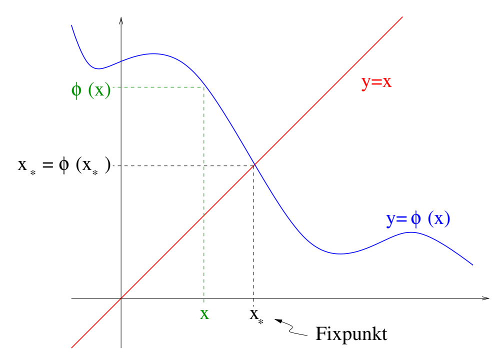
with a given function $a(x) \neq 0$. Then

$$f(x) = 0 \quad \Leftrightarrow \quad x = \phi(x).$$

In numerical mathematics: a root-finding problem is often transformed into a fix point problem

Illustration of fix point problems

Fix points of the function ϕ are the values, at which the curve $y = \phi(x)$ intersects with the curve $y = x$.



Fix point iteration (1-dimensional, i. e. in $\mathbb{R}$)

Assume a given (finite or infinite) interval $\mathcal{J} \subseteq \mathbb{R}$ and a function $\phi : \mathcal{J} \to \mathcal{J}$ (self-mapping).

Iteration sequence:

(1) Choose an initial value $x_0 \in \mathcal{J}$.

(2) Let $x_{k+1} := \phi(x_k), \quad k = 1, 2, \ldots$.

We will show: If ϕ is continuous and the iterative sequence $x_0, x_1, x_2, \ldots$ converges, then the limit of the sequence is a fix point of ϕ.

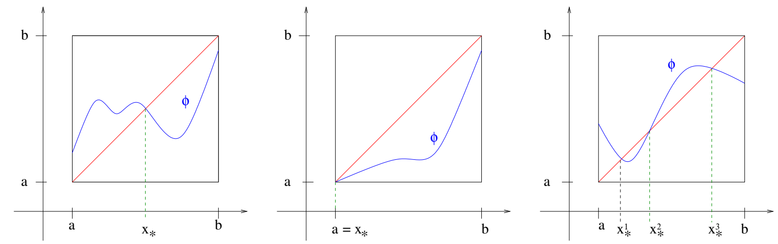
Proof: Let $x_* = \lim_{k\to\infty} x_k$. Then

$$\phi(x_*) = \phi(\lim_{k\to\infty} x_k) \underset{\substack{\uparrow \\ \text{continuity}}}{=} \lim_{k\to\infty} \phi(x_k) = \lim_{k\to\infty} x_{k+1} = \lim_{k\to\infty} x_k = x_*.$$

Fix point theorem

Let $\mathcal{J} = [a, b]$ be a finite, closed interval and let $\phi : \mathcal{J} \to \mathcal{J}$ continuous. Then ϕ has **at least** one fix point x_*.

Illustration:



Intuitive explanation of the fix point theorem: The graph of ϕ (blue curve) starts at the left side of the square and ends at the right side. The line $x = y$ (red line) divides the square into a left triangle and a right triangle. Therefore the graph of the function and the line $y = x$ intersect in at least one point.

Formal proof: The function $f(x) = \phi(x) - x$ is continuous. We have $f(a) \geq 0$ and $f(b) \leq 0$. Since f is continuous, with the mean value theorem we can conclude that at least one value x_* exist between a and b, such that $f(x_*) = 0$.

Questions:

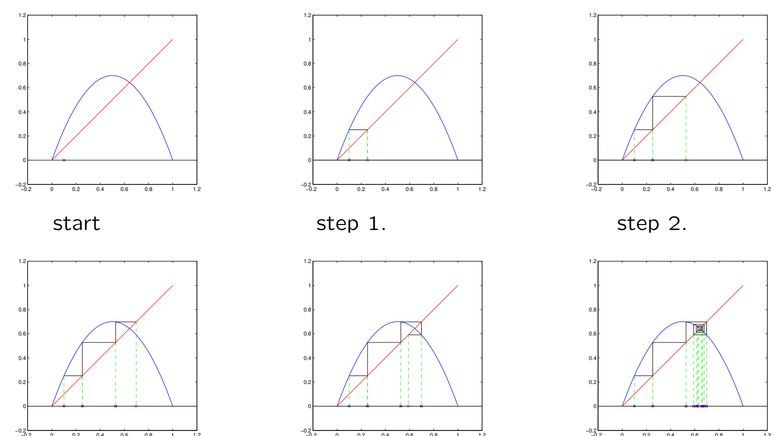
1. Assume $\phi : \mathcal{J} \to \mathcal{J}$ has exactly one fix point. Does every iteration sequence converges to this fix point?
2. Assume $\phi : \mathcal{J} \to \mathcal{J}$ has several fix points and the iteration sequence with initial value x_0 converges. Which fix point is the limit of the sequence?
3. How can we visualize a fix point iteration?

Graphical illustration of a fix point iteration

The pictures below show the fix point iteration of the function (parabola)

$$\phi_a(x) = a\,x\,(1 - x), \qquad a = 2.8.$$

The little 'x' on the x-axis are the values x_k of the iteration sequence $x_{k+1} = \phi(x_k)$ with initial value $x_0 = 0.1$. Details will be explained in the lecture.



start — step 1. — step 2. — step 3. — step 4. — step 10.

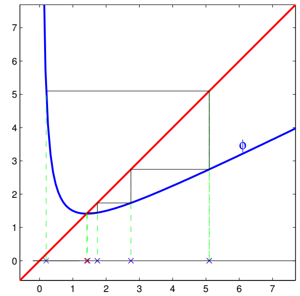
Heron-method to compute $\sqrt{a}$

Let $a > 0$ and $\phi(x) = \frac{1}{2}\left(x + \frac{a}{x}\right)$, $x > 0$.

Then the sequence converges

$$x_{k+1} = \phi(x_k) = \frac{1}{2}\left(x_k + \frac{a}{x_k}\right)$$

for every positive initial value x_0 to $\sqrt{a}$.



Proof sketch: Show (see Figure)

(1) $\sqrt{a} \le \phi(x)$ for all $x > 0$,

(2) $\phi(x) \le x$ for all $x \ge \sqrt{a}$.

(3) The only fix point of ϕ is $\sqrt{a}$.

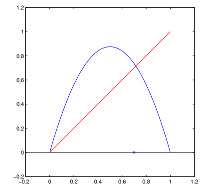
From (1) and (2) it follows that the sequence x_k is monotone decreasing at least after the second term, and the sequence is bounded from below by $\sqrt{a}$. Sequences which are monotone and bounded from below are convergent. We already showed that in general that then the limit of the sequence is a fix point of ϕ, which is here $\sqrt{a}$.

Example of a repelling fix point

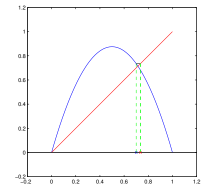
The figures below show the fix point iteration for the function (parabola)

$$\phi_a(x) = a\,x\,(1-x), \qquad a = 3.5.$$

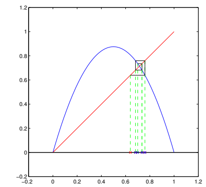
Although the initial value $x_0 = 0.7$ is close to the fix point, the iteration sequence does not converge. Already the first steps bring the terms of the sequence further away from the fix point. Such a fix point is called repellor.



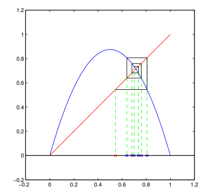
start



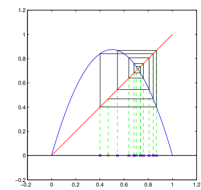
step 1.



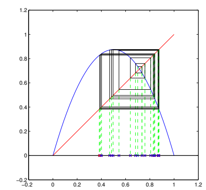
step 4.



step 7.



step 10.



step 20.

Definition of the terms attracting fix point and repelling fix point

Let $\mathcal{J}$ be an interval and let $\phi : \mathcal{J} \to \mathcal{J}$ be self-mapping.

1. A fix point x_* of ϕ is called **attracting**, if an $\epsilon > 0$ and a constant $L < 1$ exist, s. t.
$$|\phi(x) - x_*| \le L\,|x - x_*| \qquad \text{for all } x \in \mathcal{J} \cap [x_* - \epsilon, x_* + \epsilon] \qquad (*)$$
2. A fix point x_* of ϕ is called **repelling**, if an $\epsilon > 0$ and a constant $M > 1$ exist, s. t.
$$|\phi(x) - x_*| \ge M\,|x - x_*| \qquad \text{for all } x \in \mathcal{J} \cap [x_* - \epsilon, x_* + \epsilon], x \ne x_* \qquad (**)$$

Conclusions:

1. If a fix point x_* is attracting, and an iteration sequence $x_{k+1} = \phi(x_k)$ starts in the interval $\mathcal{J} \cap [x_* - \epsilon, x_* + \epsilon]$, then it converges to x_*, because from $(*)$ it follows that
$$|x_k - x_*| \le L^k\,|x_0 - x_*| \;\to\; 0.$$
2. Let x_* be a repelling fix point and let $x_k \ne x_*$ be a term of an iteration sequence which is sufficiently close to x_*. Then $(**)$ implies that
$$|x_{k+1} - x_*| \ge M\,|x_k - x_*| > |x_k - x_*|.$$
This means, that the distance between the term $x_{k+1} = \phi(x_k)$ and the fix point is greater than the distance between x_k and the fix point. $\Rightarrow$

Iterative methods cannot be used to compute (find) a repelling fix point.

When is a fix point attracting or repelling?

Theorem: Let $\phi : \mathcal{J} \to \mathcal{J}$ be self-mapping on the interval $\mathcal{J}$ which is continuous and differentiable and let x_* be a fix point of ϕ. Then:

1. If $|\phi'(x_*)| < 1$, then x_* is an attracting fix point.
2. If $|\phi'(x_*)| > 1$, then x_* is a repelling fix point.

Explanation: With the mean value theorem of calculus we get

$$\phi(x) - x_* = \phi(x) - \phi(x_*) = \int_{x_*}^{x} \phi'(x)\,dx = \phi'(\xi)\,(x - x_*).$$

$\uparrow$ mean value theorem

for a value ξ between x and x_*.Then also $|\phi(x) - x_*| = |\phi'(\xi)|\,|x - x_*|$.

<u>Conclusion:</u> For $U_\epsilon := \mathcal{J} \cap [x_* - \epsilon, x_* + \epsilon]$ and $x \in U_\epsilon$ we have

$$\underbrace{\min_{\xi \in U_\epsilon} |\phi'(\xi)|}_{M}\,|x - x_*| \le |\phi(x) - x_*| \le \underbrace{\max_{\xi \in U_\epsilon} |\phi'(\xi)|}_{L}\,|x - x_*|.$$

If $|\phi'(x_*)| < 1$ and ϵ is small enough, then also $|\phi'(\xi)| < 1$ for all $\xi \in U_\epsilon$, because ϕ' is continuous by assumption. Then also $L < 1$.
Similarly we can show that $M > 1$, if $|\phi'(x_*)| > 1$ and ϵ is small enough.

Order of convergence of a sequence

Definition:
A sequence $x_k \in \mathbb{R}$ with limit x_* **converges at least of order** $p \geq 1$ if a constant $C > 0$ and an index k_0 exist, such that

$$|x_{k+1} - x_*| \leq C\,|x_k - x_*|^p \qquad \text{für alle } k \geq k_0 \qquad (*)$$

If $p = 1$, then we say the sequence converges (at least) **linearly**. If $p = 2$, then we say the sequence converges (at least) **of second order**.

Rule: The higher the order of convergence, the faster the sequence converges.

Using the term 'linear convergence' we can define an attracting fix point as follows:

A fix point x_* of $\phi : \mathcal{J} \to \mathcal{J}$ is attracting, if every iteration sequence $x_{k+1} = \phi(x_k)$, which starts close enough to the fix point, converges at least linearly to the fix point.

Remark: The inequality $(*)$ implies already convergence, if
1) $p = 1$ and $C < 1$, or 2) $p \geq 2$ and $|x_{k_0} - x_*| < \min\{1, 1/C\}$.

Question: When does an iteration sequence have a high convergence order?

Order of convergence of an iteration sequence

Theorem: Let $\phi : \mathcal{J} \to \mathcal{J}$ be p-times continuously differentiable, where $p \geq 2$, and let x_* be a fix point of ϕ, such that

$$\phi'(x_*) = \ldots = \phi^{(p-1)}(x_*) = 0. \qquad (*)$$

Then every iteration sequence which starts close enough to x_* converges to x_* at least with order p.

Explanation: With the Taylor theorem we have

$$\phi(x) = \underbrace{\phi(x_*)}_{=x_*} + \phi'(x_*)(x - x_*) + \ldots + \frac{\phi^{(p-1)}(x_*)}{(p-1)!}(x - x_*)^{p-1} + \underbrace{\frac{\phi^{(p)}(\xi)}{p!}(x - x_*)^p}_{\text{remainder}}$$

for any value ξ between x and x_*. With $(*)$ this gives

$$\phi(x) - x_* = \frac{\phi^{(p)}(\xi)}{p!}(x - x_*)^p.$$

and also

$$|\phi(x) - x_*| \leq \underbrace{\frac{1}{p!}\max_{\xi \in U_\epsilon}|\phi^{(p)}(\xi)|}_{C}\,|x - x_*|^p,$$

where $x \in U_\epsilon := \mathcal{J} \cap [x_* - \epsilon, x_* + \epsilon]$.

Root problems and the Newton method

Problem: Find the root x_* of $f : \mathbb{R} \to \mathbb{R}$

Transform the root-finding problem into a fix point problem:
Let $a : \mathbb{R} \to \mathbb{R}$ be a function which is not zero near x_*. Let

$$\phi(x) = x + a(x) f(x)$$

Then the root x_* is a fix point of ϕ.

Question:
Can we choose the factor $a(x)$ such that we get second order convergence?

Answer: Let $a(x) = -\frac{1}{f'(x)}$, then

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

and

$$\phi'(x_*) = 1 - \frac{f'(x_*)f'(x_*) - f(x_*)f''(x_*)}{f'(x_*)^2} = 0$$

which gives convergence of second order.

However, this requires:
f is 2-times continuously differentiable near x_* and $f'(x_*) \neq 0$.

The iterative method with the function $(*)$ is called Newton method.

Another derivation of the Newton method

Problem: Find the root x_* of $f : \mathbb{R} \to \mathbb{R}$

Assume that we know that the root x_* is close to $x_0 \in \mathbb{R}$.
Then we have $x_* = x_0 + h$ with a small correction h. With Taylor we have

$$0 = f(x_*) \;=\; f(x_0 + h) \;=\; f(x_0) + f'(x_0)\,h + o(h).$$

Ignorring the remainder $o(h)$ and reorder/solve for h gives

$$h \approx -\frac{f(x_0)}{f'(x_0)}, \qquad \text{also} \qquad x_* = x_0 + h \approx x_0 - \frac{f(x_0)}{f'(x_0)}$$

We define the right side of this approximative equation as x_1:

$$x_1 := x_0 - \frac{f(x_0)}{f'(x_0)}.$$

x_1 is (hopefully) a better approximation to x_* than x_0. To get and even better approximation, we repeat the method and by this we get the iteration sequence

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

Geometrical Interpretation of the Newton method:

x_{k+1} is the root of the line tangent to f at the position value x_k (see next slide).

On the geometrical interpretation of the Newton method

Taylor expansion of f at x_k:

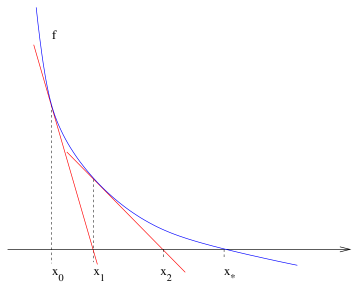
$$f(x) = f(x_k) + f'(x_k)(x - x_k) + o(x - x_k)$$

Equation for line tangent to f at x_k:

$$T(x) = f(x_k) + f'(x_k)(x - x_k)$$

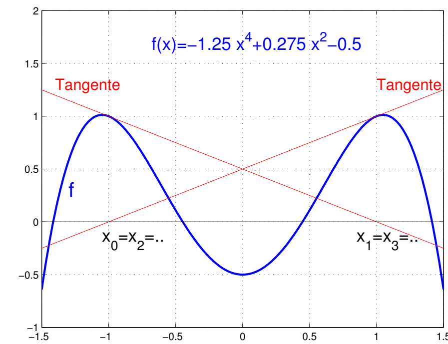
Root of the tangent line:

$$x_{k+1} := x_k - \frac{f(x_k)}{f'(x_k)} \qquad \Leftrightarrow \qquad T(x_{k+1}) = 0.$$



The Newton iteration does not always converge

Here is an example where a Newton-sequence oscillates between 2 points:



A Newton sequence can also diverge to ∞.

Another unpleasant case: After k steps we arrived at an x_k with $f'(x_k) = 0$.
Then we cannot compute the next term of the sequence $x_{k+1} = x_k - f(x_k)/f'(x_k)$.
(Geometrically: The tangent line at x_k is parallel to the x-axis)

A sufficient condition for convergence of the Newton method

Theorem:
Let f be a real valued function defined at least in the interval $\mathcal{J} = [x_0 - \epsilon, x_0 + \epsilon]$ and let f be 2-times continuously differentiable. Assume $f'(x) \neq 0$ for all $x \in \mathcal{J}$, and a constant $0 < L < 1$ exist such that

$$\left|\frac{f(x_0)}{f'(x_0)}\right| \leq (1 - L)\epsilon, \qquad \left|\frac{f(x)\, f''(x)}{f'(x)^2}\right| \leq L \quad \text{for all } x \in \mathcal{J}.$$

Then the Newton-sequence

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

with the initial value x_0 converges with order 2 to the unique root $x_* \in \mathcal{J}$ of f.

Proof: This follows from Banach's fix point theorem (see slides for the next lecture).

Note: The conditions of this theorem are not sufficient, but also not necessary.
The Newton-sequence can converge even if these conditions are not satisfied.

Other root-finding methods

The simplest, but relatively slow, method to find the roots of a function f in an interval, is the

Bisection method

<u>*Input:*</u> $a, b \in \mathbb{R}$, $a < b$, such that $f(a)$ and $f(b)$ have different signs.

Set $\ell = a$, $r = b$

Repeat as long as $r - \ell > tol$:

Set $x_k = \frac{\ell + r}{2}$ $\qquad$ (*)
If $f(x_k)$ and $f(\ell)$ have the same sign, set $\ell = x_k$.
Otherwise set $r = x_k$

Regula Falsi

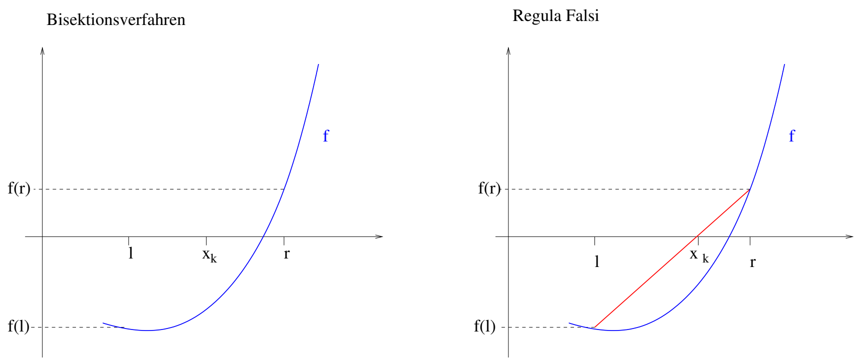
If we replace the entry condition in the Bisection method by $|x_{k+1} - x_k| > tol$ and $(*)$ by

$$x_k = \frac{\ell\, f(r) - r\, f(\ell)}{f(r) - f(\ell)}, \qquad (**)$$

we get the Regula-Falsi-method.

x_k in $(**)$ is the root of the (secant) line through the points $(\ell, f(\ell))$ and $(r, f(r))$ (see Figure on the next slide).

Figure on Bisection method and Regula Falsi



Both methods assume that the function f changes sign at the root.

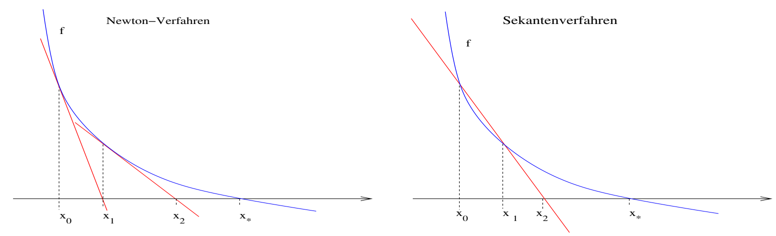
Secant method

To compute the root of a function f with the Secant method we set

$$\begin{aligned} x_{k+1} &:= \text{intersection of the line through } (x_k, f(x_k)) \text{ and } (x_{k-1}, f(x_{k-1})) \\ & \text{(secant) with the } x\text{-axis} \\ &= \frac{x_k f(x_{k-1}) - x_{k-1} f(x_k)}{f(x_{k-1}) - f(x_k)} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} = x_k - \frac{f(x_k)}{\frac{f(x_k)-f(x_{k-1})}{x_k - x_{k-1}}} \end{aligned}$$

The Secant method needs two initial values. If f is continuously differentiable and the derivative at the root is $\neq 0$, the Secant method converges, if the initial values are close enough to the root, with order of convergence $p = \frac{1+\sqrt{5}}{2}$ (golden ratio), i. e. slower than Newton.

Advantage of the secant method: No need to compute derivatives.



Newton method:

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

Secant method:

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

Newton method and Secant method in $\mathbb{C}$

Everything we said so far about iterative methods (except for the Bisection method and Regula Falsi) is true also for functions $\phi : \mathbb{C} \to \mathbb{C}$ and $f : \mathbb{C} \to \mathbb{C}$ (repelling and attracting fix points, order of convergence, etc.).
However, we cannot illustrate these methods geometrically.

The iteration step for the Newton- and Secant method to find the roots of a complex function is the same as for real functions:

Newton method:

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

Secant method:

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

But now the sequence terms x_k are in general complex numbers, i. e. points in the complex plane.

Important application: Finding roots of polynomials.

Example: Find the third root of one

The equation $x^3 = 1$ has the complex solutions (=third root of 1)

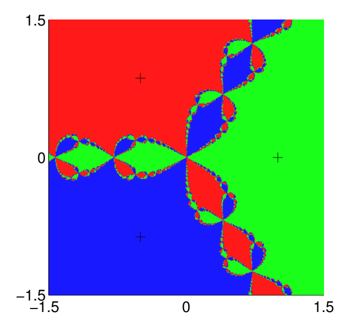
$$x_1^* = 1, \qquad x_2^* = \frac{-1 + \sqrt{3}\,i}{2}, \qquad x_3^* = \frac{-1 - \sqrt{3}\,i}{2}.$$

The iteration step for the Newton method is

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \qquad \text{where } f(x) = x^3 - 1.$$

To which root the sequence converges (or if it diverges, or if it ends due to division by zero), depends on the initial value x_0:

x_0 in the green area $\Rightarrow$ convergence to x_1^*
x_0 in the red area $\Rightarrow$ convergence to x_2^*
x_0 in the blue area $\Rightarrow$ convergence to x_3^*



All three areas share a common boundary (cannot be seen in the picture). If we chose a boundary point as initial value, then the Newtonsequence does not converge.

Examples of iterations in $\mathbb{C}$:
Julia-sets and the Mandelbrot-sets (apple man)

Let $z, c \in \mathbb{C}$. Consider the sequence

$$x_{k+1} = x_k^2 + c, \qquad x_0 = z \qquad (*)$$

Julia-set

$$J_c := \{\, z \in \mathbb{C} \mid \text{ The sequnce } (*) \text{ is bounded } \}$$

Mandelbrot-set:

$$\begin{aligned} M &:= \{\, c \in \mathbb{C} \mid \text{ the set } J_c \text{ is connected } \} \\ &= \{\, c \in \mathbb{C} \mid \text{ the sequence } x_{k+1} = x_k^2 + c,\ \ x_0 = 0, \text{ ist is bounded } \} \end{aligned}$$

See `http://astronomy.swin.edu.au/ pbourke/fractals/juliaset/`