# NUMERICAL SOLUTION OF INITIAL VALUE PROBLEMS



## Introduction



### Examples

• Motion of a pendulum ( $\phi(0) = \alpha$ )

$$\phi'(t) = \pm \sqrt{\frac{2g}{l}} \sqrt{\cos \phi(t) - \cos \alpha}$$

 (Alfred James) Lotka (1925, USA) - (Vito) Volterra (1926, Italian) predator-pray model (u(0), v(0) are given)

$$u'(t) = u(t)(2 - v(t)),$$
  
 
$$v'(t) = v(t)(u(t) - 1).$$

• Deflection of a rod (y(0) = y(L) = 0)

$$EIy''(x) + P\cos(y(x)) = 0.$$

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The first two examples are so-called initial value problems, while the third one is a so-called boundary value problem.

### Initial value problems

 $\overline{\mathbf{y}}' = \mathbf{f}(x, \overline{\mathbf{y}}), \quad \overline{\mathbf{y}}(x_0) \text{ adott}$ 

where  $\overline{\mathbf{y}}: [a, b] \to \mathbb{R}^n$  is the unknown function,  $\mathbf{f}: [a, b] \times \mathbb{R}^n \to \mathbb{R}^n$ , moreover  $x_0 \in [a, b]$ .

Other forms:

$$\overline{\mathbf{y}}'(x) = \mathbf{f}(x, \overline{\mathbf{y}}(x)),$$

or componentwise

$$y'_1(x) = f_1(x, y_1, \dots, y_n),$$
  
$$\vdots$$
  
$$y'_n(x) = f_n(x, y_1, \dots, y_n),$$

Order of the equation: the highest order of the derivative of the unknown function that appear in the equation.

### Initial value problems

Example. Higher order equations with one unknown can be rewritten to a system of ordinary differential equations. In case of

$$y'' + 3y'y + xy = 0$$
,  $y(x_0), y'(x_0)$  given

we can rewrite the equation as

$$y_1'(x) = y_2, \quad y_1(x_0) \text{ given} \\ y_2'(x) = -xy_1 - 3y_2y_1, \quad y_2(x_0) \text{ given}.$$

Solution: A function  $\overline{y}$  that is differentiable sufficiently many times, fulfils the initial condition and if we substitute it back into the equation then we arrive at an identity.

### Existence and uniqueness

#### Rudolf Otto Sigismund Lipschitz (1832 - 1903, German)

**Def. 134.** We say that the function  $\mathbf{f} : [a, b] \times \mathbb{R}^n \to \mathbb{R}^n$  is Lipschitz continuous in its second argument, if  $\exists L \geq 0$  such that for all  $x \in [a, b]$  and  $\overline{\mathbf{z}}_1, \overline{\mathbf{z}}_2 \in \mathbb{R}^n$  we have

$$\|\mathbf{f}(x,\overline{\mathbf{z}}_1) - \mathbf{f}(x,\overline{\mathbf{z}}_2)\| < L\|\overline{\mathbf{z}}_1 - \overline{\mathbf{z}}_2\|.$$

Thm. 135. If the right hand side function **f** of the initial value problem

$$\overline{\mathbf{y}}' = \mathbf{f}(x, \overline{\mathbf{y}}), \quad \overline{\mathbf{y}}(a)$$
 given

is continuous in its first argument on [a, b] and Lipschitz continuous in its second argument then the problem has a unique solution, which is continuously differentiable.

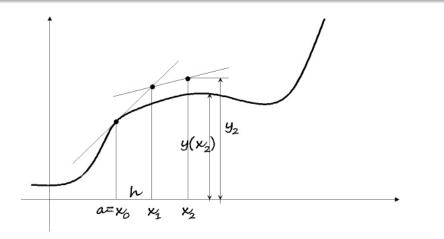
# Explicit Euler method



## Explicit Euler method (EE)

The method was published by Euler in a three-volume book between 1768 and 1770.

 $y'(x) = f(x, y(x)), \quad y(x_0)$  given.



We define a mesh on the interval  $[x_0, x_{max}]$  and we approximate the value of the solution function only at these points.

The mesh is  $x_k = x_0 + hk$   $(k = 0, 1, ..., N_h)$ , where h is an arbitrary positive step size.  $N_h$  is the maximum positive integer that satisfies  $hN_h \leq x_{\text{max}}$ . Let us denote the approximations in the mesh points by  $\overline{y}_k$ .

The the formula of the Explicit Euler method is:

 $\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + h\mathbf{f}(x_k, \overline{\mathbf{y}}_k), \quad \overline{\mathbf{y}}_0 \text{ is known from } \overline{\mathbf{y}}(x_0).$ 

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**Def. 136.** The iteration formula that prescribes how to calculate the approximation values at the mesh points is called numerical scheme (or method).

The general numerical schemes we will deal with have the form

$$\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + h\Phi(h, x_k, \overline{\mathbf{y}}_{k+1}, \overline{\mathbf{y}}_k, \dots, \overline{\mathbf{y}}_{k+1-s}),$$

where  $\Phi$  is the so-called increment function (EE-case:  $\Phi = \mathbf{f}(x_k, \overline{\mathbf{y}}_k)$ ), and s is a positive integer. Notice that the other mesh points can be expressed with  $x_k$  and h.

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## General notions of the numerical methods of ODEs

**Def. 137.** A numerical scheme (or method) is explicit, if  $\Phi$  is independent of  $\overline{\mathbf{y}}_{k+1}$ , that is we do not need to solve equations to get  $\overline{\mathbf{y}}_{k+1}$ . Otherwise the scheme is implicit.

**Def. 138.** The number s is called the number of steps of the scheme. The scheme is called one-step scheme (method) if s = 1 (only the data at the kth point are used to the approximation at the (k + 1)th point). The scheme is a multistep scheme if s > 1.

Example. The EE (scheme) method is a one-step explicit (scheme) method.

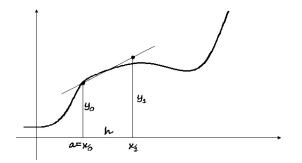
In the sequel we will investigate one-step methods only. The multistep methods are considered in a separate section.

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# Implicit Euler and Crank–Nicolson methods



## Implicit Euler method (IE)



The scheme is

$$\overline{\mathbf{y}}_k = \overline{\mathbf{y}}_{k+1} - h\mathbf{f}(x_{k+1}, \overline{\mathbf{y}}_{k+1}),$$

where we have to solve a non-linear system of equations in each iteration step. This can be solved e.g. with fixed point iteration starting from the estimate in the previous point  $\overline{y}_k$ .

Rmk. The implicit Euler method is a one-step implicit method.

## Crank–Nicolson method (CN, trapezoidal)

#### John Crank (1916 - 2006), Phyllis Nicolson (1917 - 1968), English.



The scheme

$$\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + \frac{h}{2}(\mathbf{f}(x_k, \overline{\mathbf{y}}_k) + \mathbf{f}(x_{k+1}, \overline{\mathbf{y}}_{k+1})).$$

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This is also a one-step implicit scheme.

## Other derivations

#### Numerical integration:

$$y'(x) = f(x,y) \Rightarrow \int_{x_0}^{x_0+h} y'(x) \, \mathrm{d}x = \int_{x_0}^{x_0+h} f(x,y(x)) \, \mathrm{d}x$$

#### Thus

$$y(x_0 + h) - y(x_0) = \int_{x_0}^{x_0 + h} f(x, y(x)) \, \mathrm{d}x$$

$$\approx \begin{cases} f(x_0, y_0)h, & (EE) \\ f(x_0 + h, y(x_0 + h))h, & (IE) \\ (f(x_0, y_0) + f(x_0 + h, y(x_0 + h)))h/2 & (CN). \end{cases}$$

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### Other derivations

#### Numerical differentiation:

We change the derivative with the forward difference approximation.

$$\frac{y(x_0 + h) - y(x_0)}{h} \approx f(x_0, y(x_0)),$$

After rearrangement we arrive at the scheme of the EE method.

#### Taylor's method

$$y(x_0+h) = y(x_0) + \underbrace{y'(x_0)}_{f(x_0,y(x_0))} h + \frac{y''(x_0)h^2}{2} + \frac{y'''(x_0)h^3}{6} + etc.$$

When we stop after the first order term, then we get the EE scheme. If we can compute the derivatives of function f(x, y) with respect to x, then we can produce the Taylor's series of the solution to arbitrary order.

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### The $\theta$ -method

Let  $\theta \in [0,1]$  be an arbitrary parameter and let us consider the numerical integration formula

$$y(x_0 + h) - y(x_0) = \int_{x_0}^{x_0 + h} f(x, y(x)) \, \mathrm{d}x$$
  
 
$$\approx h(\theta f(x_0 + h, y(x_0 + h)) + (1 - \theta) f(x_0, y(x_0))).$$

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#### Special cases:

- The  $\theta = 0$  case gives the EE scheme,
- the  $\theta = 1$  case gives the IE scheme,
- and the  $\theta = 1/2$  case gives the CN scheme.

# Consistency, stability, convergence



## A numerical experiment (EE method)

#### Example.

$$y'(x) = \frac{y(x) + x}{y(x) - x}, \quad y(0) = 1.$$

Exact solution

$$y(x) = x + \sqrt{1 + 2x^2}.$$

$$h = \frac{1}{k} | y_1 - y(x_1) | y_k - y(1)$$

$$\frac{1}{2} -0.2247 -0.2321$$

$$\frac{1}{4} -0.0607 -0.1065$$

$$\frac{1}{8} -0.0155 -0.0510$$

$$\frac{1}{16} -0.0039 -0.0249$$

The error is second order at the first mesh point and first order at the point x = 1.

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### Convergence

Let  $\overline{\mathbf{e}}_k$  denote the difference  $\overline{\mathbf{y}}_k - \overline{\mathbf{y}}(x_k)$   $(k = 0, \dots, N_h)$ .

Def. 139. A numerical scheme (method) is said to be convergent, if

$$\max_{k=1,\dots,N_h} \|\overline{\mathbf{e}}_k\| = O(h^r)$$

 $(r \ge 1)$ , and we say that the order of the convergence is (at least) r.

**Def. 140.** Local truncation error (LTE): the remainder when we pretend that the exact solution satisfies the scheme is written in the form  $h\tau_{k+1}$ .  $\tau_{k+1}$  is called the local truncation error at the point  $x_{k+1}$ .

Example. For one-step schemes we have

$$\overline{\mathbf{y}}(x_{k+1}) = \overline{\mathbf{y}}(x_k) + h\Phi(h, x_k, \overline{\mathbf{y}}(x_k), \overline{\mathbf{y}}(x_{k+1})) + h\boldsymbol{\tau}_{k+1}.$$

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### Consistency

Example. Computation of the local truncation error for the EE method ( $\overline{\mathbf{y}} \in C^2$ ):

$$\boldsymbol{\tau}_{k+1} = \frac{\overline{\mathbf{y}}(x_{k+1}) - \overline{\mathbf{y}}(x_k)}{h} - \mathbf{f}(x_k, \overline{\mathbf{y}}(x_k))$$
$$= \frac{\overline{\mathbf{y}}(x_k) + \overline{\mathbf{y}}'(x_k)h + \overline{\mathbf{y}}''(\xi_k)h^2/2 - \overline{\mathbf{y}}(x_k)}{h} - \mathbf{f}(x_k, \overline{\mathbf{y}}(x_k))$$
$$= \overline{\mathbf{y}}''(\xi_k)h/2.$$

Thus, all local truncation errors are bounden by  $M_2h/2$ .

**Def. 141.** If all the truncation errors are bounded by  $Ch^r$  ( $C \ge 0$  constant and  $r \ge 1$ ), then the numerical scheme is called consistent with the order of consistency r.

Example. The EE method ( $\overline{\mathbf{y}} \in C^2$ ) is consistent with consistency order 1.

**Def. 142.** A numerical scheme is called to be (zero-)stable on the interval  $[x_0, x_{\text{max}}]$  if there are numbers K > 0 (independent of h) and  $h_0 > 0$  such that

$$\max_{k=1,\dots,N_h} \|\overline{\mathbf{y}}_k - \overline{\mathbf{z}}_k\| \le K \|\overline{\mathbf{y}}_0 - \overline{\mathbf{z}}_0\|$$

if  $0 < h < h_0$ . ( $\overline{\mathbf{z}}_k$  is a vector sequence starting from  $\overline{\mathbf{z}}_0$  and defined by the numerical scheme.)



### Convergence

**Thm. 143.** (The equivalence theorem.) Let us suppose that the order of the consistency of a numerical scheme is  $r \ge 1$ . Then the necessary and sufficient condition of the convergence is the stability. The order of the convergence is r.

Thm. 144. Let us consider the initial value problem

$$\overline{\mathbf{y}}' = \mathbf{f}(x, \overline{\mathbf{y}}), \quad \overline{\mathbf{y}}(x_0) \text{ given}$$

with a solution  $\overline{\mathbf{y}} \in C^2$ . Then the explicit Euler method is convergent and the convergence order is 1, moreover we have

$$\|\overline{\mathbf{e}}_k\| \le e^{(x_{\max}-x_0)L}h(x_{\max}-x_0)M_2/2.$$

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### Convergence

**Proof**. We prove only the stability, which gives the convergence due to the equivalence theorem.

We start from two arbitrary vector sequences that are generated by the explicit Euler scheme

$$\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + h\mathbf{f}(x_k, \overline{\mathbf{y}}_k),$$
$$\overline{\mathbf{z}}_{k+1} = \overline{\mathbf{z}}_k + h\mathbf{f}(x_k, \overline{\mathbf{z}}_k).$$

We subtract the two equalities and use the Lipschitz continuity of the function f.

$$\|\overline{\mathbf{y}}_{k+1} - \overline{\mathbf{z}}_{k+1}\| = \|\overline{\mathbf{y}}_k - \overline{\mathbf{z}}_k\| + h\|\mathbf{f}(x_k, \overline{\mathbf{y}}_k) - \mathbf{f}(x_k, \overline{\mathbf{z}}_k)\| \le \\ \le \|\overline{\mathbf{y}}_k - \overline{\mathbf{z}}_k\| + hL\|\overline{\mathbf{y}}_k - \overline{\mathbf{z}}_k\| \le (1 + hL)\|\overline{\mathbf{y}}_k - \overline{\mathbf{z}}_k\|.$$

Thus we have

$$\|\overline{\mathbf{y}}_k - \overline{\mathbf{z}}_k\| \le (1 + hL)^k \|\overline{\mathbf{y}}_0 - \overline{\mathbf{z}}_0\| \le e^{khL} \|\overline{\mathbf{y}}_0 - \overline{\mathbf{z}}_0\| = e^{(x_{\max} - x_0)L} \|\overline{\mathbf{y}}_0 - \overline{\mathbf{z}}_0\|.$$

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This estimation shows the stability of the scheme.

### Convergence of the $\theta$ method

Thm. 145. Let us consider the initial value problem

$$\overline{\mathbf{y}}' = \mathbf{f}(x, \overline{\mathbf{y}}), \quad \overline{\mathbf{y}}(x_0)$$
 given

 $(\overline{\mathbf{y}} \in C^3)$ . Then the  $\theta$  method is convergent and

$$\left\|\overline{\mathbf{e}}_{k}\right\| \leq \frac{h}{4} \left( \left| \frac{1}{2} - \theta \right| M_{2} + \frac{h}{3} M_{3} \right) \left( e^{\frac{(b-a)L}{1-\theta Lh}} - 1 \right),$$

where  $M_3 = \max_{x \in [a,b]} \|\overline{\mathbf{y}}'''(x)\|$ .

Rmk. The Crank–Nicolson method has second order, while the other methods are only first order convergent.

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#### Carl David Tolmé Runge (1856 - 1927, German), Martin Wilhelm Kutta (1867 - 1944, German)



Let us assume that f is sufficiently smooth. Then the solution  $\overline{y}$  will be also sufficiently smooth. Let us expand  $\overline{y}$  into Taylor series at the point  $x_0$ :

$$\overline{\mathbf{y}}(x_0+h) = \overline{\mathbf{y}}(x_0) + h \underbrace{\overline{\mathbf{y}}'(x_0)}_{=\mathbf{f}(x_0,\overline{\mathbf{y}}(x_0))} + \frac{h^2}{2} \underbrace{\overline{\mathbf{y}}''(x_0)}_{=?} + \dots$$

 $\overline{\mathbf{y}}''(x_0)$  can be calculated, but we need the derivatives of  $\mathbf{f}$ .

$$\overline{\mathbf{y}}''(x_0) = \mathbf{f}'_x(x_0, \overline{\mathbf{y}}(x_0)) + \mathbf{f}'_y(x_0, \overline{\mathbf{y}}(x_0))\mathbf{f}(x_0, y(x_0)).$$

Thus

$$\overline{\mathbf{y}}(x_0 + h) = \overline{\mathbf{y}}(x_0) + h \left( \mathbf{f}(x_0, \overline{\mathbf{y}}(x_0)) + \frac{h}{2} \left( \mathbf{f}'_x(x_0, \overline{\mathbf{y}}(x_0)) + \mathbf{f}'_y(x_0, \overline{\mathbf{y}}(x_0)) \mathbf{f}(x_0, \overline{\mathbf{y}}(x_0)) \right) \right) + \dots$$

Let us search for a sufficiently accurate approximation of the highlighted factor in the form

$$a\mathbf{f}(x_0, \overline{\mathbf{y}}(x_0)) + b \underbrace{\mathbf{f}(x_0, \overline{\mathbf{y}}(x_0)) + \mathbf{f}'_x(x_0, \overline{\mathbf{y}}(x_0)) \alpha h + \mathbf{f}'_y(x_0, \overline{\mathbf{y}}(x_0)) \beta h \mathbf{f}(x_0, \overline{\mathbf{y}}(x_0)) + O(h^2)}_{\mathbf{f}(x_0, \overline{\mathbf{y}}(x_0)) + \mathbf{f}'_x(x_0, \overline{\mathbf{y}}(x_0)) \alpha h + \mathbf{f}'_y(x_0, \overline{\mathbf{y}}(x_0)) \beta h \mathbf{f}(x_0, \overline{\mathbf{y}}(x_0)) + O(h^2)},$$

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where  $a, b, \alpha, \beta$  are suitable real constants.

We obtain that

$$a+b=1, \quad \alpha b=\beta b=rac{1}{2},$$

and writing all parameters as functions of b we obtain

$$a = 1 - b, \quad \alpha = \beta = \frac{1}{2b}.$$

General form:

 $\overline{\mathbf{y}}_{k+1}$ 

$$=\overline{\mathbf{y}}_k + h((1-b)\mathbf{f}(x_k,\overline{\mathbf{y}}_k) + b\mathbf{f}(x_k+h/(2b),\overline{\mathbf{y}}_k + \mathbf{f}(x_k,\overline{\mathbf{y}}_k)h/(2b))).$$

Rmk. The consistency order of these methods ( $b \neq 0$ ) is 2. It can be proven that they are also stable. Thus these methods are convergent and the order of the convergence is 2.

Rmk. Special cases:

Modified Euler method (RK2, b = 1):

$$\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + h\mathbf{f}(x_k + h/2, \overline{\mathbf{y}}_k + \mathbf{f}(x_k, \overline{\mathbf{y}}_k)h/2).$$

Simplified Runge–Kutta or Heun method (b = 1/2):

$$\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + h\left(\mathbf{f}(x_k, \overline{\mathbf{y}}_k)/2 + \mathbf{f}(x_k + h, \overline{\mathbf{y}}_k + \mathbf{f}(x_k, \overline{\mathbf{y}}_k)h)/2\right) + \mathbf{f}(x_k, \overline{\mathbf{y}}_k)h(x_k, \overline{$$

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### Runge-Kutta methods - general form

 $\overline{\mathbf{y}}_{k+1} = \overline{\mathbf{y}}_k + h\Phi(x_k, \overline{\mathbf{y}}_k, h),$ 

where

$$\Phi(x, \overline{\mathbf{y}}, h) = \sum_{r=1}^{R} c_r k_r$$

and

$$k_{1} = \mathbf{f}(x, \overline{\mathbf{y}}),$$

$$k_{r} = \mathbf{f}(x + ha_{r}, \overline{\mathbf{y}} + h\sum_{s=1}^{r-1} b_{rs}k_{s}), \quad r = 2, \dots, R,$$

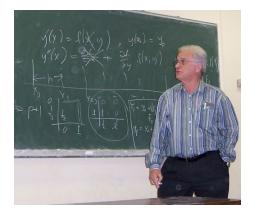
$$a_{r} = \sum_{s=1}^{r-1} b_{rs}, \quad r = 2, \dots, R.$$

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R is called the number of the stages of the method.

### Runge-Kutta methods - Butcher's tableau

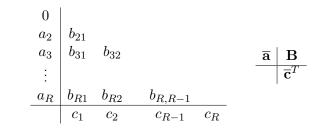
The coefficients can be conveniently written in a tabular form (so-called Butcher's tableau).



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John C. Butcher (1933 -, New-Zealand)

### Runge-Kutta methods - Butcher's tableau



The consistency order of the methods (the conditions are understood cumulatively):

cons. order	condition		
1	$\overline{\mathbf{a}} = \mathbf{B}\overline{\mathbf{e}}  \overline{\mathbf{c}}^T\overline{\mathbf{e}} = 1$		
2	$\overline{\mathbf{c}}^T \overline{\mathbf{a}} = 1/2$		
3	$\overline{\mathbf{c}}^T(\overline{\mathbf{a}}^{\cdot 2}) = 1/3  \overline{\mathbf{c}}^T \mathbf{B}\overline{\mathbf{a}} = 1/6$		
4	$\overline{\mathbf{c}}^T(\overline{\mathbf{a}}^{\cdot 3}) = 1/4$ $\overline{\mathbf{c}}^T$ diag $(\overline{\mathbf{a}})\mathbf{B}\overline{\mathbf{a}} = 1/8$		
	$\overline{\mathbf{c}}^T \mathbf{B}(\mathbf{a}^{\cdot 2}) = 1/12  \overline{\mathbf{c}}^T \mathbf{B}^2 \overline{\mathbf{a}} = 1/24$		

Runge-Kutta methods - RK2, Heun, RK4 methods

Example. Modified Euler (RK2) and Heun methods (two-stage methods):

Rmk. The achievable highest order with fixed number of stages:

number of stages $(m)$	1, 2, 3, 4	5, 6, 7	8, 9, 10
max. order	m	m-1	m-2

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### Runge-Kutta methods - RK2, Heun, RK4 methods

Example. Fourth order (four-stage) Runge–Kutta method (RK4):

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# Absolute stability



### The test problem

Let us applied the studied methods to the initial value problem

$$y' = \lambda y, \quad y(0) = 1,$$

where  $\lambda < 0$  is an arbitrary negative real number.

The solution is  $y(x) = e^{\lambda x}$ , which converges to 0 as  $x \to \infty$ .

**Def. 146.** If a numerical method with a fixed step size h is applied to the test problem and the numberical solution  $|y_k|$  tends to 0 as  $k \to \infty$  then the method is called absolute stable.

Naturally, the absolute stability depends on both  $\lambda$  and h.

**Def. 147.** The set  $\mathcal{A} = \{z = h\lambda \in \mathbb{R} \mid \text{the method is absolute stable with } z\}$  is called the domain of absolute stability. If  $\mathbb{R}^- \subset \mathcal{A}$ , then the method is called to be A-stable.

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### Absolute stability of the EE and IE methods

#### EE method:

$$y_k = (1 + h\lambda)^k,$$

which tends to zero only if  $|1 + h\lambda| < 1$ , that is if  $z = h\lambda$  lies in a circle with radius 1 and with center at -1.

The method is absolute stable iff  $h < -2/\lambda$ .

IE method:

$$y_k = \frac{1}{(1 - h\lambda)^k},$$

which tends to zero only if  $z = h\lambda$  lies in a circle with radius 1 and with center at 1. The method is A-stable.

Rmk. None of the (explicit) Runge-Kutta methods are A-stable.

# Solution of stiff equations



The high stability of the equations results in instability in the numerical solution. Equations for which implicit methods work well and explicit methods behave badly. Equations for which the choice of h is restricted not by the accuracy but by the absolute stability.

Example. The efficient solution of the van der Pol equation ( $\mu = 100000$ ):

$$y'_1 = y_2$$
  
 $y'_2 = \mu(1 - y_1^2)y_2 - y_1;$ 

Example. The solution of the equation y' = -15y + 1, y(0) = 0.