

TMA4125 Matematikk 4N

Numerics for Initial Value Problems

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Motivation

Similar to Integration: Only a very limited number of ODEs can be solved analytically.

Example. A simple pendulum

$$\begin{cases} \theta''(t) &= -\frac{g}{L}\sin(\theta(t))\\ \theta(0) &= \theta_0\\ \theta'(0) &= 0 \end{cases}$$

has no analytical solution!

Approximate for small θ : sin $\theta \approx \theta$ \Rightarrow We can solve the approximate ODE

$$\theta'' = -\frac{g}{L}\theta \quad \Leftrightarrow \quad \theta(t) = \theta_0 \cos\left(\sqrt{\frac{g}{L}}t\right), \quad \text{period } T = \frac{2\pi}{\sqrt{gL}} = 2\pi\sqrt{\frac{L}{g}}.$$



First Order ODEs

A scalar ODE of first order is an equation of the form

 $y'(t) = f(t, y(t)), \qquad y(t_0) = y_0$

where $y'(t) = \frac{dy}{dt}$ and $y(t_0) = y_0$ is required for uniqueness.

These ODEs are called initial value problems (IVP). We are interested in the solution y(t) for $t > t_0$ If f depends linearly on y it is called linear.

Examples.

- ▶ y'(t) = 3y(t), f(t, y) = 3y, linear
- ▶ y'(t) = -2ty(t), f(t,y) = -2ty, linear
- ▶ $y'(t) = t^3 2t^2y(t)$, $f(t, y) = t^3 2t^2y$, linear
- ▶ $y'(t) = 1 (y(t))^2$, $f(t, y) = 1 y^2$, nonlinear

Systems of ODEs

A System of ODEs is given by

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$$y'_1 = f_1(t, y_1, y_2, \dots, y_m), \qquad y_1(t_0) = y_{1,0}$$

 $y'_2 = f_2(t, y_1, y_2, \dots, y_m), \qquad y_2(t_0) = y_{2,0}$

$$y'_m = f_m(t, y_1, y_2, \dots, y_m), \qquad y_m(t_0) = y_{m,0}$$

or more compactly

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t)), \qquad \mathbf{y}(t_0) = \mathbf{y}_0$$

with

$$\mathbf{y}(t) = \begin{pmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_m(t) \end{pmatrix}, \quad \mathbf{f}(t, \mathbf{y}) = \begin{pmatrix} f_1(t, y_1, y_2, \dots, y_m) \\ f_2(t, y_1, y_2, \dots, y_m) \\ \vdots \\ f_m(t, y_1, y_2, \dots, y_m) \end{pmatrix}, \quad \mathbf{y}_0 = \begin{pmatrix} y_{1,0} \\ y_{2,0} \\ \vdots \\ y_{m,0} \end{pmatrix}$$

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Example: Preditor-Prey or Lotka-Volterra-Model We describe 2 species

- $y_1(t)$ is the population of some prey (maybe rabbits, or small fish)
- $y_2(t)$ is the population of some predator (maybe foxes or sharks)

Then we have a (simplified) model of their interaction as

$$y_1'(t) = \alpha y_1(t) - \beta y_1(t)y_2(t) y_2'(t) = \delta y_1(t)y_2(t) - \gamma y_2(t)$$

where $\alpha,\beta,\delta,\gamma$ are parameters describing the interaction. Or in short

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t))$$
 with $\mathbf{f}(t, \mathbf{y}) = \begin{pmatrix} \alpha y_1 - \beta y_1 y_2 \\ \delta y_1 y_2 - \gamma y_2 \end{pmatrix}$

Notes.

We need some initial populations \mathbf{y}_0 and some initial time t_0 But. The right hand side does not depend on t



Autonomous ODEs

A (system of) ODE(s) is called autonomous if the function f only depends on y and not (directy) on t

▶ y'(t) = 3y(t), f(t, y) = 3y, autonomous, linear

▶
$$y'(t) = -2ty(t)$$
, $f(t,y) = -2ty$, non-autonomous, linear

▶
$$y'(t) = 1 - (y(t))^2$$
, $f(t, y) = 1 - y^2$, autonomous, nonlinear

A trick. A system of ODEs, can be made autonomous introducing a m + 1st variable

$$y'_{m+1} = 1, \qquad y_{m+1}(t_0) = t_0$$

and replacing all occurrences of t in f by y_{m+1} .



Higher Order ODEs

An initial value problem (IVP) for an ODE of order m is given by

$$u^{(m)} = f(t, u, u', \dots, u^{(m-1)}),$$

$$u(t_0) = u_0,$$

$$u'(t_0) = u'_0,$$

$$\vdots$$

$$u^{(m-1)}(t_0) = u_0^{(m-1)}$$

where $u^{(1)} = u'$ and $u^{(m+1)} = \frac{\mathrm{d}u^{(m)}}{\mathrm{d}t}$ for m > 0 denotes the (m+1)st derivative.

Rewrite.

We can rewrite a higher order ODE into a system of first-order ODEs.



Higher order ODEs to System of ODEs

Introduce. New variables: $y_1(t) = u(t)$, $y_2(t) = u'(t)$, $y_3(t) = u^{(2)}(t)$,..., $y_m(t) = u^{(m-1)}(t)$.

We observe. Taking the derivative $y'_i = (u^{(i+1)})' = u^{(i+2)} = y_{i+1}$, i = 1, ..., m - 1. \Rightarrow We obtain the following first order **System** of ODEs

$$y'_{1} = y_{2}$$

$$y'_{2} = y_{3}$$

$$\vdots$$

$$y'_{m-1} = y_{m}$$

$$y'_{m} = f(t, y_{1}, y_{2}, y_{3}, \dots, y_{m}))$$



Example. Van der Pol's Equation

Van der Pol's equation is a second order differential equation given by

$$u'' = \mu(1 - u^2)u' - u,$$
 $u(0) = u_0,$ $u'(0) = u'_0,$

where $\mu > 0$. Common choices. $u_0 = 2$, $u'_0 = 0$.

System of First Order ODEs

$$y'_1 = y_2 y_1(0) = u_0 y'_2 = \mu(1 - y_1^2)y_2 - y_1 y_2(0) = u'_0$$



Numerical Methods



Terms and Notation

Focus. Scalar ODEs, but can be directly applied to systems of ODEs, too.

Approach. We will take timesteps $t_0, t_1, t_2, ...$ introduce/compute the approximations $y_n \approx y(t_n)$. \Rightarrow for "errors" we consider $|y_n - y(t_n)|!$

Methods. We will only consider one-step methods. Given

- ▶ an ODE (i.e. a right hand side *f*)
- ▶ initial values (t_0, y_0)
- ► a step size *h*
- \Rightarrow We compute a first step $y_1 \approx y(t_1)$ with $t_1 = t_0 + h$
- \Rightarrow based on (t_1, y_1) : compute $y_2 \approx y(t_2)$ with $t_2 = t_1 + h$
- ... and so on until a final time t_{end} is reached.



One-Step Methods and Beyond

One-Step Methods are only "allowed" to use the information from the previous step,

i.e. the approximation y_{k+1} does not depend on $y_{k-1}, y_{k-2}, ...$

Main alternative. multi-step methods are allowed to take previous values into account as well.

Summary. We numerically compute an approximation to y at discrete time points t_n , n = 0, 1, ...,

Be careful! We often compare

- $y(t_n)$ the (analytical) solution at t_n
- y_n the *n*th step of the numerical methods (which only approximates $y(t_n)$)



Euler's method

A first algorithm to solve $\mathbf{y}' = \mathbf{f}(t, \mathbf{y})$ is given as¹

Euler's method

- **1.** Given / Input: A function f(t, y) and initial value (t_0, y_0)
- **2.** Choose a step size h
- **3.** For $n = 0, 1, 2 \dots$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n)$$
$$\mathbf{t}_{n+1} = t_n + h$$

Let's look at two examples in Python.

¹either derived via Taylor expansion or forward differences



Trapezoidal method

Idea. Let's integrate the ODE $\mathbf{y}'(t) = \mathbf{f}(t, y)$ from t_n to t_{n+1} . And use the trapezoidal rule to approximate the integral

The update for the Trapezoidal rule reads

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{h}{2} \big(\mathbf{f}(t_n, \mathbf{y}_n) + \mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}) \big).$$

This is a so-called implicit method, since y_{n+1} appears on boths sides and is hence only implicitly given.

 \Rightarrow We would have to solve for \mathbf{y}_{n+1} in every iteration.



Heun's method

Remedy. Instead of solving the nonlinear equation for y_{n+1} , first approximate/replace y_{n+1} on the right by applying a step from Euler's method. We obtain

Heun's method.

$$\mathbf{u}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n)$$
$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{h}{2} \big(\mathbf{f}(t_n, \mathbf{y}_n) + \mathbf{f}(t_{n+1}, \mathbf{u}_{n+1}) \big).$$

This is more commonly written (emphasizing reusing terms) as

$$\mathbf{k}_1 = \mathbf{f}(t_n, \mathbf{y}_n),$$

$$\mathbf{k}_2 = \mathbf{f}(t_n + h, \mathbf{y}_n + h\mathbf{k}_1),$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{h}{2}(\mathbf{k}_1 + \mathbf{k}_2).$$

Notation Interlude: Increment function Φ

We saw that the one-step methods can be written as

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_n \mathbf{\Phi}(t_n, \mathbf{y}_n, \mathbf{y}_{n+1}, h_n),$$

where for us $h_n = h$ does not change during the iterations (but it indeed could), and The function Φ is called increment function.

A method is called

- explicit if $\mathbf{\Phi}$ does not depend on \mathbf{y}_{n+1}
- implicit if $\mathbf{\Phi}$ does depend on \mathbf{y}_{n+1}

Examples. Are the following implicit or explicit?

- ▶ Euler: $\mathbf{\Phi}(t_n, \mathbf{y}_n, \mathbf{y}_{n+1}, h) = \mathbf{f}(t_n, \mathbf{y}_n)$
- ► Trapezoidal: $\Phi(t_n, \mathbf{y}_n, \mathbf{y}_{n+1}, h) = \frac{1}{2} (\mathbf{f}(t_n, \mathbf{y}_n) + \mathbf{f}(t_n + h, \mathbf{y}_{n+1}))$
- Heun: $\Phi(t_n, \mathbf{y}_n, \mathbf{y}_{n+1}, h) = \frac{1}{2} (\mathbf{f}(t_n, \mathbf{y}_n) + \mathbf{f}(t_n + h, \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n)))$



Runge-Kutta

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Runge-Kutta-Method

Definition. An *s*-stage Runge-Kutta method is given by

$$\mathbf{k}_{i} = \mathbf{f}(t_{n} + c_{i}h, \ \mathbf{y}_{n} + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_{j}), \qquad i = 1, 2, \dots, s$$
$$\mathbf{y}_{n+1} = \mathbf{y}_{n} + h\sum_{i=1}^{s} b_{i}\mathbf{k}_{i}$$

Defined by its coefficients, which are given in a Butcher tableau

 \Rightarrow THe method is explicit if $a_{ij} = 0$ for $j \ge i$ (diagonal and above).

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Examples of Runge-Kutta Euler.

0 0

Heun.

 $\begin{array}{cccc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$

Trapezoidal.

0	0	0
1	$\frac{1}{2}$	$\frac{1}{2}$
	$\frac{1}{2}$	$\frac{1}{2}$

RK4	I.			
0	0	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	0
$\frac{\frac{1}{2}}{\frac{1}{2}}$	0	$\frac{1}{2}$	0	0
1	0	0	1	0
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$



Theoretical Results



Motivation.

We want to be able to tell

- When does a solution exist?
- When is a solution unique?
- How large is the error one step introduces?
- How large can the global (overall) error get?
- ► How does the error behave depending on the step size *h*?

In other words: While we do not have the exact solution y(t), we still want to be able to say how close we are to that, so what the error is in our computations, and how much is needed to improve/reduce it.



Lipschitz condition

Definition. A function $\mathbf{f} : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ satisfies a Lipschitz condition with respect to \mathbf{y} on a domain $(a, b) \times D$ where $D \subset \mathbb{R}^m$ if there exists a constant L such that

$$\|\mathbf{f}(t, \mathbf{y}) - \mathbf{f}(t, \mathbf{z})\| \le L \|\mathbf{y} - \mathbf{z}\|, \quad \text{for all} \quad t \in (a, b) \text{ and } \mathbf{y}, \mathbf{z} \in D$$

holds.

The constant *L* is called the Lipschitz constant.

Remark. \mathbf{f} is Lipschitz if

- if $\frac{\partial f_i}{\partial y_j}$, i, j = 1, ..., m are continuous and bounded on $(a, b) \times D$
- D is open and convex



Existence of solutions

Theorem (Existence and uniqueness of a solution) *Consider the initial value problem*

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \qquad \mathbf{y}(t_0) = \mathbf{y}_0$$

with given initial values $t_0 \in (a, b)$ and $\mathbf{y}_0 \in D$.

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• $\mathbf{f}(t, \mathbf{y})$ is continuous in $(a, b) \times D$

f (t, \mathbf{y}) satisfies the Lipschitz condition with respect to \mathbf{y} in $(a, b) \times D$, then the ODE has one and only one solution in $(a, b) \times D$.

In the following we assume that our ODE under consideration fulfils this.



Error Analysis

When we aplve an ODE e.g. with Euler's method on $[t_0, t_{end}]$ we can ask ourselves

- How will the error at the end t_{end} (or any point in between) depend on the number of steps?
- ▶ phrased differently: Choose N and set $h = \frac{t_{end} t_0}{N}$. Then we get $t_N = t_{end}$. What can we say about the error $e_N = y(t_{end} - y_N)$?

In the following we will just consider the scalar equation y' = f(t, y). The results also hold for systems of equations.

Local and Global Error

We will consider two types of errors:

- ► Local Truncation Error (LTE) d_{n+1} denotes the error made in one single step starting from the exact/true point $(t_n, y(t_n))$
- Global error e_n

denotes the difference between the exact ($y(t_n)$) and numerical (y_n) solution after n steps:

$$e_n = y(t_n) - y_n$$

Goals.

- find an expression for d_n
- look at the relation between local errors and the global error
- find an upper bound for the global error



Local Truncation Error for Euler's method

Investigating the error in one step for an ODE y' = f(t, y). From the Taylor expansion we get

$$y(t_n + h) = y(t_n) + hy'(t_n) + \frac{1}{2}y''(\xi), \qquad t_n < \xi < t_n + h$$

Eulers method starting from $(t_n, y(t_nT))$ yields

$$y(t_n + h) \approx y(t_n) + hf(t_n, y(t_n)) = y(t_n) + hy'(t_n)$$

 \Rightarrow The local truncation error for Euler's method: their difference

$$d_{n+1} = y(t_n + h) - (y(t_n) + hy'(t_n)) = \frac{1}{2}h^2 y''(\xi), \qquad \xi \in (t_m, t_n + h)$$

We can observe two things

- with a bound *C* for $y''(\xi)$ yields that $d_{n+1} = \mathcal{O}(h^2)$
- see the error of Euler's method in: $y(t_n + h) = y(t_n) + h(f(t_n, y_n)) + d_{n+1}$



Global Error for Euler's Scheme

Summary.

We have the exact step (inculding d_{n+1}) and the numerical scheme

$$y(t_n + h) = y(t_n) + hf(t_n, y(t_n)) + d_{n+1}$$

$$y_{n+1} = y_n + hf(t_n, y_n)$$

Goal. Using

$$\blacktriangleright \ e_n = y(t_n) - y_n$$

- ▶ an upper bound for $f_y = \frac{\partial f}{\partial y}$ as $|f_y(t, y)| \le L$ (a Lipschitz constant)
- ▶ an upper bound for $|y''(t)| \le 2D$

find

- **1.** an upper bound for $|e_{n+1}|$
- **2.** by iteration an upper bound for $|e_N|$
- \Rightarrow We want to say something about decreasing h or increasing N and how e_N behaves then.



Global Error for Euler's Scheme – Result

We obtain

$$|y(t_{
m end})-y_N|=|e_N|\leq Dh\leq Ch,$$
 where $C=rac{{
m e}^{L(t_{
m end}-t_0)}-1}{L}D$ depends on

- ▶ the length of our interval $t_{end} t_0$
- certain properties of y (the D) and f (the L)
- ! but not on N or h!

We especially get

$$\lim_{N \to \infty} |e_N| = 0$$

Remark.

- We got locally $d_{n+1} = \mathcal{O}(h^2)$
- We got globally $e_N = \mathcal{O}(h)$

Roughly speaking because it takes N (in order of $\frac{1}{N}$) steps (with local errors) to "reach" t_{end} .

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Local Truncation Error & Consistency

For a Numerical method to solve the ODE y' = f(t, y) we consider the Increment function Φ (again), that is, the function that describes our numerical method as

$$y_{n+1} = y_n + h\Phi(t_n, y_n, h)$$

then the local truncation error reads as

$$d_{n+1} = y(t_n + h) - (y(t_n) + h\Phi(t_n, y(t_n), h)).$$

Definition (Consistency)

A numerical method is called consistent if

$$\lim_{h \to 0} \frac{d_{n+1}}{h} = 0, \qquad \text{for all } n = 0, 1, \dots, N, N = \left\lceil \frac{b-a}{h} \right\rceil$$

It is called consistent of order p if $d_{n+1} = \mathcal{O}(h^{p+1})$.



Remark on Consistency

For systems of equations

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{\Phi}(t_n, \mathbf{y}_n, h)$$

by considering the absolute norm of the LTE, i. e. if

$$\|\mathbf{y}(t+h) - (\mathbf{y}(t) + h\mathbf{\Phi}(t, \mathbf{y}(t), h))\| \le Dh^{p+1}$$

then numerical method for the system of ODEs is consistent of order *p*.

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Convergence

Theorem (Convergence of one-step methods)

Assume that there exist positive constants M and D such that the increment function Φ satisfies

$$\|\mathbf{\Phi}(t, \mathbf{y}, h) - \mathbf{\Phi}(t, \mathbf{z}, h)\| \le M \|\mathbf{y} - \mathbf{z}\|$$

and the method is consistent of oder p, that is the local truncation error satisfies

$$\|\mathbf{y}(t+h) - (\mathbf{y}(t) + h\mathbf{\Phi}(t,\mathbf{y}(t),h))\| \le Dh^{p+1}$$

for all t, y and z in a neighbourhood of the solution. In that case, the global error satisfies

$$\|\mathbf{e}_N\| = \|\mathbf{y}(t_{\text{end}}) - \mathbf{y}_N\| \le Ch^p, \quad \text{with } C = \frac{e^{M(t_{\text{end}} - t_0)} - 1}{M}D.$$

The method is then called (convergent) of order p.

Remarks on Convergence

We saw. Consistency (of order p) and Lipschitz condition \Rightarrow Convergence (of oder p).

Example. For Euler's method: $\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n)$ $\Rightarrow \mathbf{\Phi}(t, \mathbf{y}, h) = \mathbf{f}(t, \mathbf{y}).$ $\Rightarrow L = M$ is the same constant

For Runge-Kutta Methods. The corresponding increment function Φ is maybe complicated a constant M as required in the Theorem always exists.



Convergence Order for Runge-Kutta

For Runge-Kutta methods, one can prove:

The method is of order p with $p \le 4$ if all of the conditions in the table on the left up to and including p are fulfilled. (all sums run from 1 to s.)

Remark.

Similar conditions for higher order exist, but get a bit more complicated.

Example. Let's check Heun's method.

p	conditions
1	$\sum_i b_i = 1$
2	$\sum_i b_i c_i = 1/2$
3	$\sum_i b_i c_i^2 = 1/3$
	$\sum_{i,j} b_i a_{ij} c_j = 1/6$
4	$\sum_i b_i c_i^3 = 1/4$
	$\sum_{i,j} b_i c_i a_{ij} c_j = 1/8$
	$\sum_{i,j} b_i a_{ij} c_j^2 = 1/12$
	$\sum_{i,j,k} b_i a_{ij} a_{jk} c_k = 1/24$

Summary (including systems of Equations) Notation / Definitions.

- ► the ODE: $\mathbf{y}' = \mathbf{f}(t, \mathbf{y})$
- the exact solution through (t^*, \mathbf{y}^*) : $\mathbf{y}(t, t^*, \mathbf{y}^*)$
- the exact solution of the ODE with initial values t_0 , y_0 :

 $\mathbf{y}(t) = \mathbf{y}(t\,;\,t_0,\mathbf{y}_0)$

• one step of the (explicit) method (increment function Φ):

 $\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{\Phi}(t_n, \mathbf{y}_n, h)$

Error Concepts.

Let $\mathbf{\Phi}$ represent a method of order p and $\hat{\mathbf{\Phi}}$ a method of order p+1.

- ► local truncation error (LTE) (comparing exact solution to one step "from there"): $\mathbf{d}_{n+1} = \mathbf{y}(t_n + h; t_n, \mathbf{y}(t_n)) - (\mathbf{y}(t_n) + h\mathbf{\Phi}(t_n, \mathbf{y}(t_n), h))$
- ► local error: $\mathbf{l}_{n+1} = \mathbf{y}(t_n + h; t_n, \mathbf{y}_n) (\mathbf{y}_n + h\mathbf{\Phi}(t_n, \mathbf{y}_n, h))$

• the global error:
$$\mathbf{e}_n = \mathbf{y}(t_n) - \mathbf{y}_n$$

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Error Estimates & Adaptivity

Motivation

In our numerical tests we saw that the step size h has to be chosen

- if it is too large \Rightarrow too inexact results in \mathbf{y}_n
- if it is too small \Rightarrow too much computational time or memory usage

Approaches.

- **1.** control the global error $\mathbf{e}_n = \mathbf{y}(t_n) \mathbf{y}_n$ this is quite difficult and beyond the scope of this lecture
- **2.** control the local error $\mathbf{l}_{n+1} \coloneqq \mathbf{y}(t_{n+1}; t_n, \mathbf{y}_n) \mathbf{y}_{n+1}$ where
 - we "start from" (t_n, \mathbf{y}_n) : We consider the exact solution $\mathbf{y}(t; t_n, \mathbf{y}_n)$ but running through (t_n, \mathbf{y}_n) .
 - compared to d_{n+1} we have hence a "different starting point" y_n and not y(t_n)!



Approximating the local error

Recap. We saw that for the convergence order we needed power serieses in *h*.

Now since we do not have the actual solution $\mathbf{y}(t)$, let's take two methods, where one is more exact. For both we start from our previous point (t_n, \mathbf{y}_n) :

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{\Phi}(t_n, \mathbf{y}_n, h)$$
$$\hat{\mathbf{y}}_{n+1} = \mathbf{y}_n + h\hat{\mathbf{\Phi}}(t_n, \mathbf{y}_n, h)$$