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Chapter 7.1, 7.2 and 7.3.

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The numerical approximation $(x_1, x_2, \ldots, x_n)$ is

- an approximation of the unknown solution $x(t)$, and
- only given at discrete t-values $t_i = t_0 + ih, \quad i = 1, \ldots, n$:

$$x_0 \approx x(t_0), x_1 \approx x(t_1), \ldots, x_n \approx x(t_n).$$

Partial Differential Equations (with more independent variables $t, y, \ldots$) are introduced e.g. in the course 01418 and their numerical methods in 02686, 02687, 02689.

Higher-order differential equation $\longrightarrow$ system of first order

Numerical solvers are **only** for systems of first-order differential equations.

A single differential equation of order n,

$$\frac{d^n x}{dt^n} = f\left(t, x, \frac{dx}{dt}, \ldots, \frac{d^{(n-1)}x}{dt^{(n-1)}}\right),$$

can be turned into a system of n first-order equations of the form

$$\frac{d\boldsymbol{z}(t)}{dt} = \boldsymbol{f}\left(t, \boldsymbol{z}(t)\right).$$

It requires n auxiliary conditions (e.g. initial conditions) in order to specify the solution precisely.

Initial values problems

Example:

$$\frac{dx}{dt} = -3x$$

Initial values problems

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$$\frac{dx}{dt} = -3x$$

$x(t) = ke^{-3t}$ for any $k \in \mathbb{R}$.

With an extra condition, e.g. $x(0) = 7$, a unique solution is determined:

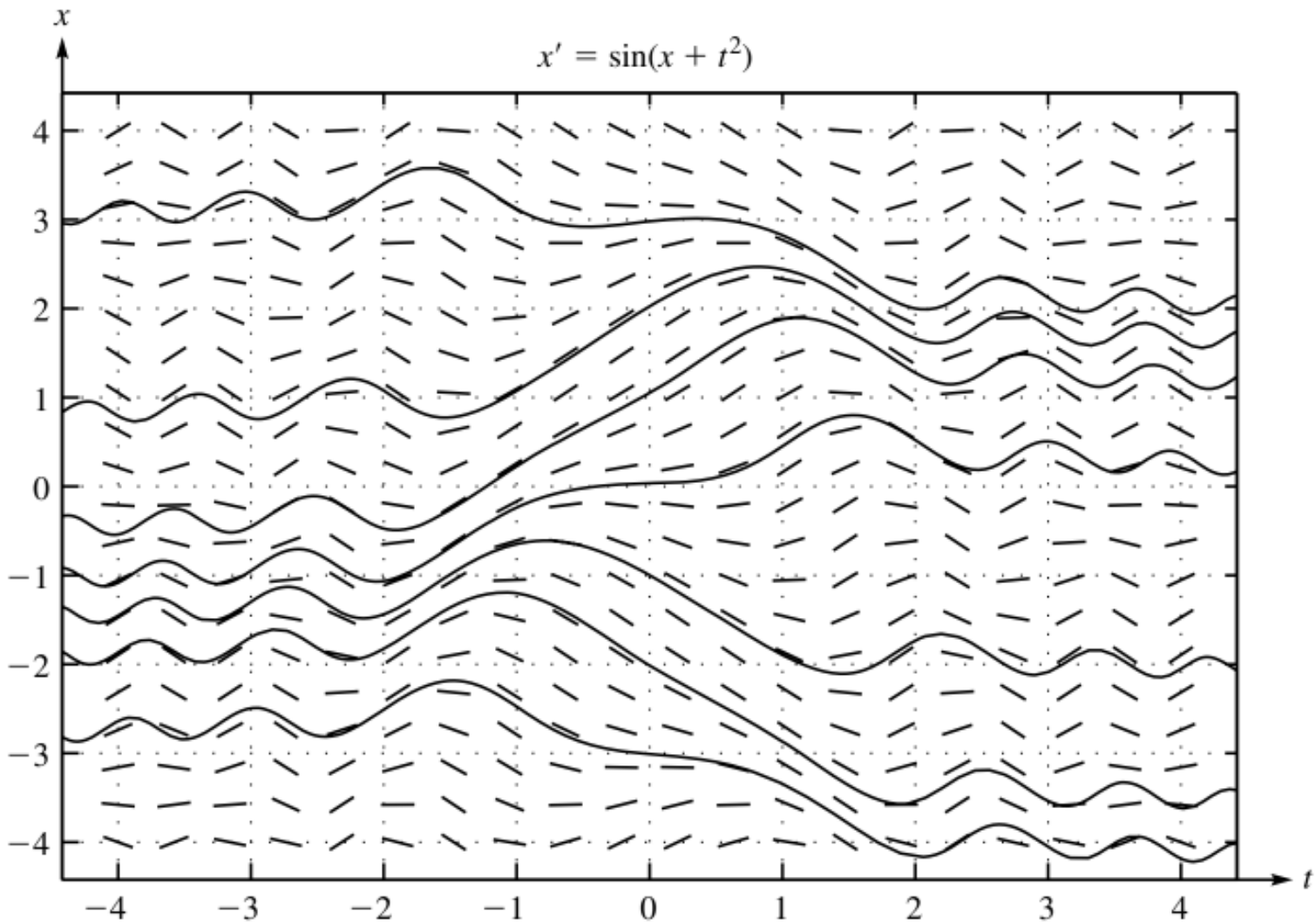
$$x(t) = 7e^{-3t}, \quad t \in \mathbb{R}.$$

Initial-value problems (this week):

$$\frac{d\,x(t)}{dt} = f\big(t, x(t)\big), t > t_0, \qquad \text{with } x(t_0) = x_0.$$

Vector fields

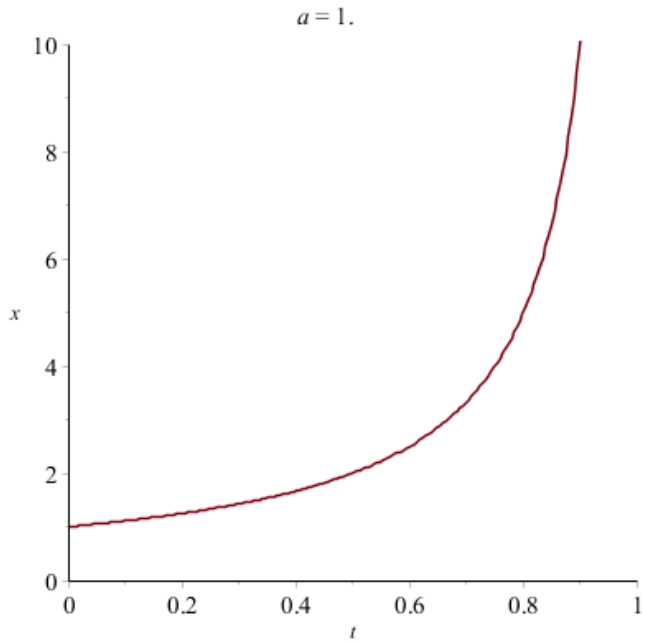
$$x' = f(x,t) = \sin(x + t^2)$$



Existence and uniqueness of solutions

Theorem:

If f is differentiable, then the initial value problem has a unique solution for $x(t)$ defined for $t \in (t_0, t_0 + \epsilon)$.



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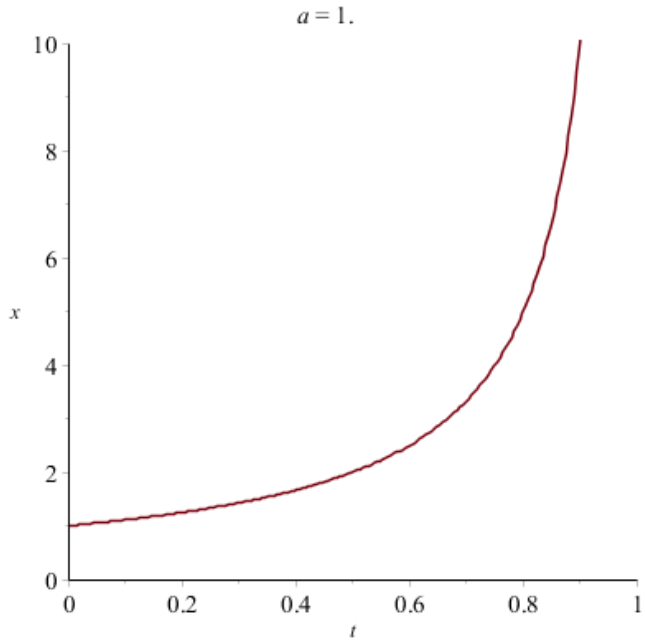
Example: For $a > 0$ the solution to

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

is

$$x(t) = \frac{1}{(1 - at)^{\frac{1}{a}}}.$$



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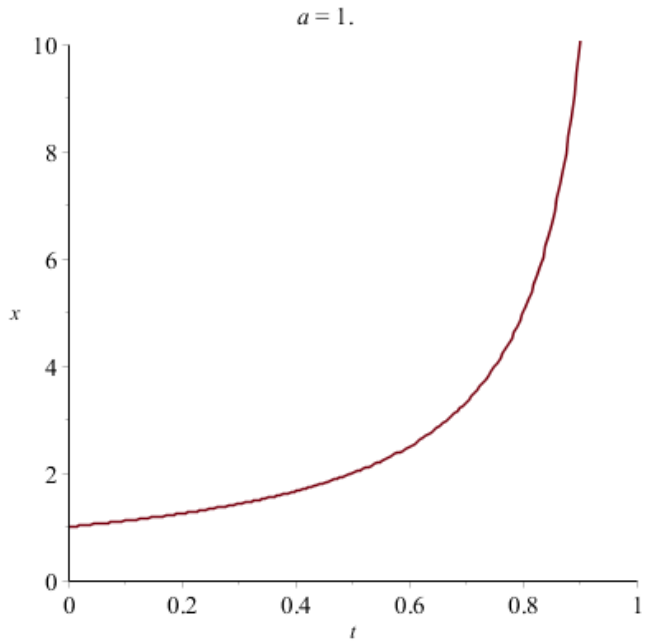


But the solution exists only as $t < \frac{1}{a}$.

Note: Numerical studies requires an idea about which time interval makes sense to look for a solution in.

Euler's method – one step

Consider the initial-value problem

$$\frac{d\,x(t)}{dt} = f\big(t, x(t)\big), \;\; x(a) = x_a.$$

The second order Taylor polynomium for x around t is

$$x(t+h) \approx x(t) + hx'(t) = x(t) + hf\Big(t, x(t)\Big).$$

Plugging in $t = t_0$ we approximate $x(t+h)$ by Euler's formula

$$x(t+h) \approx x_1 = x_0 + hf\Big(t, x_0\Big).$$

Note that x_1 is obtained from x_0 by following the slope field $f(t, x)$.

Euler's method – more steps

Now split the interval $[a, b]$ into n subintervals with size $h = (b - a)/n$. Euler's method starts from $x(a) = x_a$ and after n steps

$$\begin{aligned} x_0 &= x(a) = x_a \rightarrow \\ x_1 &\approx x(a + h) \rightarrow \\ x_2 &\approx x(a + 2h) \rightarrow \\ &\cdots \rightarrow \\ x_n &\approx x(a + nh) = x(b) \end{aligned}$$

ending with an approximation of $x(b)$.

- Euler's method is not commonly used in practice. But it's good for illustration.
- The following methods can be considered as generalized Euler's method.
- Have a look at `MyEuler.py` and `TestEuler.py`

Taylor series methods

Euler's method only uses $f\big(t, x(t)\big) = x'(t)$.
If we have higher order derivatives, e.g.

$$x''(t) = \frac{d\, f\big(t, x(t)\big)}{dt} = f'_t(t,x) + f'_x(t,x)x' = \frac{df}{dt}\big(t, x, x'\big),$$
$$x'''(t) = \cdots = \frac{d^2 f}{dt^2}\big(t, x, x', x''\big),$$

then based on Taylor series we can obtain better approximation

Taylor series methods of the first/second/third order are:

```
dx=f(t,x)                                  % given by user
d2x=dfdt(t,x,dx)                           % given by user
d3x=d2fdt2(t,x,dx,d2x)                     % given by user
x=x+h*dx                          % Euler's method; the 1st order
x=x+h*(dx+1/2*h*(d2x))                          %  2nd order
x=x+h*(dx+1/2*h*(d2x+1/3*h*(d3x)))              % 3rd order
```

Taylor series methods

When we use Taylor series method of order k, only the terms up to order k in Taylor series of $x(t)$ are included, which leads to a *local truncation error*

$$\frac{1}{(k+1)!}x^{(k+1)}(\xi)h^{k+1}, \quad \text{some } \xi \in (a,b)$$

in each iteration.

But how is the local error accumulated to a global error?

We will give an estimate for Euler's method later today, and show a numerical experiment.

Taylor series methods

- It's easy to understand
- It's easy to implement.
- But ....

Taylor series methods

- It's easy to understand
- It's easy to implement.
- But .... the user need provide

$$f(t,x), \frac{df}{dt}(t,x,x'), \frac{d^2f}{dt^2}(t,x,x',x''), \ldots$$

- Then some other tools can be needed, e.g.
  - symbolic differentiation (like Maple) or
  - automatic differentiation (a program that "differentiates another program")
- Methods that **only** use $f(t,x)$ are preferred.

Heun's method and midpoint method

Heun's method and midpoint method

Both methods shown on the board can be written in the form:

$$\begin{aligned} K_1 &= f(t, x) \\ K_2 &= f(t + \alpha h, x + \beta h K_1) \\ x(t + h) &= x(t) + h * \left(\omega_1 K_1 + \omega_2 K_2\right) \end{aligned}$$

Such methods are called Runge-Kutta methods.

NB: In the book, the notations are defined as

$$K_1 = h\, f(t, x) \text{ and } K_2 = h\, f(t + \alpha h, x + \beta K_1).$$

Error estimation for Runge-Kutta methods of order 2

In `RungeKuttaOrden2Fejlestimat.mw` it shows all terms up to second order in the Taylor series of exact solution equals the Runge-Kutta approximation if the following conditions are satisfied:

$$1 = \omega_1 + \omega_2$$
$$\frac{1}{2} = \omega_2 \alpha$$
$$\frac{1}{2} = \omega_2 \beta$$

Hence, the error in each iteration is $\mathcal{O}(h^3)$ or $\mathcal{O}(1/n^3)$.

That is, the local error is proportional to h^3 or to $1/n^3$ for a small value of h or a large value of n.

For Euler's method, the local error is $\mathcal{O}(h^2)$.

Global error estimation for Runge-Kutta methods of order 2

Initial values problem:

$$\frac{d\,x(t)}{dt} = f\big(t, x(t)\big), \;\; x(a) = x_a, \;\; \text{for} \;\; t \in [a, b].$$

- Split the interval $[a, b]$ into n subintervals with size $h = (b - a)/n$ and use a Runge-Kutta method n times.
- This gives the estimation x_i of $x(t_i)$ at the discrete time $t_i = a + ih$.

$$x(a) = x_0 \to x_1 \to x_2 \to \cdots \to x_n \approx x(b)$$

- There are n local errors, and every error is 'proportional' to h^3 and to $1/n^3$.
- Bound: The global error is 'proportional' to h^2 and to $1/n^2$.
- For Euler's method, the local error is $\mathcal{O}(h^2)$. Then is the global error $\mathcal{O}(h^1)$?

Let's try!

Example

Consider the initial values problem

$$\frac{dx}{dt} = t^2 - 2x, \;\; x(0) = x_0 = 1, \;\; t \in [0, 1],$$

which has the exact solution $x(t) = \frac{1}{4} + t\left(-\frac{1}{2} + \frac{1}{2}t\right) + \frac{3}{4}e^{-2t}$.

Here we assess the accuracy of the numerical solution by checking the relative error at the end point in the interval

$$\left| \frac{x_{\text{numerical}}(1) - x(1)}{x(1)} \right| = \left| \frac{x_n - x(1)}{x(1)} \right|.$$

NB: You also can use other error measures.

Example

The 2nd-order methods need two function evaluations in each iteration; so we count the total number of function evaluations, n_f, and compare the relative error:

n_f	n_{order1}	n_{order2}	*Euler*	*Midpoint*	*Heun*
10	10	5	0.1231	0.0367	0.0519
20	20	10	0.0606	0.0079	0.0113
40	40	20	0.0301	0.0018	0.0027
80	80	40	0.0150	0.0004	0.0006

The 2nd-order methods give better accuracy with the same effort!

For Euler's method the global error is reduced to half, when n is doubled, while for 2nd-order methods the global error is divided by 2^2.

Their global errors are $\mathcal{O}(1/n)$ and $\mathcal{O}(1/n^2)$, respectively – equals to the sum of the local errors.

Runge-Kutta methods of order 4

One commonly used 4th-order method is:

$$x(t+h) = x(t) + \frac{h}{6}\Big(K_1 + 2K_2 + 2K_3 + K_4\Big)$$

where

$$\begin{aligned} K_1 &= f(t, x) \\ K_2 &= f(t + {}^{h}/_{2}, x + {}^{h}/_{2}K_1) \\ K_3 &= f(t + {}^{h}/_{2}, x + {}^{h}/_{2}K_2) \\ K_4 &= f(t + h, x + hK_3). \end{aligned}$$

NB: Again, in the book it defines $K_1 = hf(t, x)$..., but we follow the same notations as in Chapter 7.4.

Runge-Kutta methods of order 4

The derivation of the Runge-Kutta formulas of order 4 follows that the solution at $x(t+h)$ agrees with the Taylor expansion up to and including the term in h^4. Hence, the local error is $\mathcal{O}\left(1/n^5\right)$.

Therefore, the global error is $\mathcal{O}\left(1/n^4\right)$.

In general, Runge-Kutta methods of order k have local error $\mathcal{O}\left(1/n^{(k+1)}\right)$ and global error $\mathcal{O}\left(1/n^k\right)$.

Adaptive methods

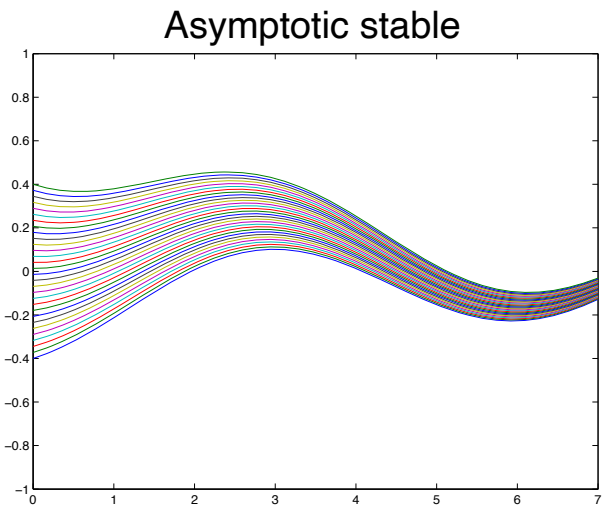
Similar as in integration, it's interesting to develop new methods such that the step size depending on the right-hand side of ODE.

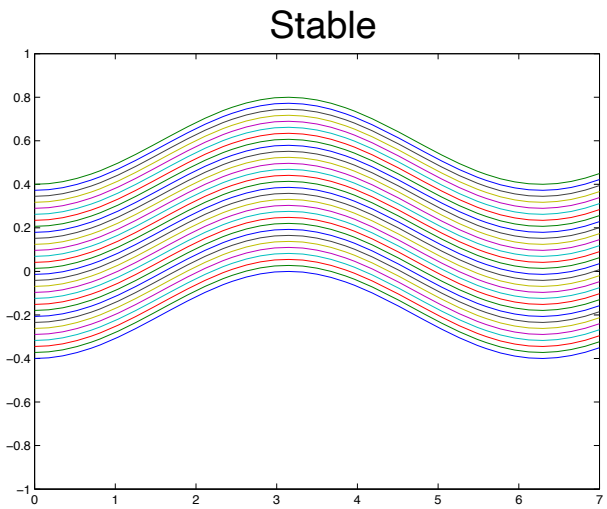
There is a widely used algorithm which is also implemented in the scipy.integrate package: `solve_ivp`. By default, it uses RK45, which based on the computation of 6 derivatives, calculates both a 4th and a 5th order Runge-Kutta method. It also gives an error estimate that can be used for an adaptive procedure. See Chapter 7.3.

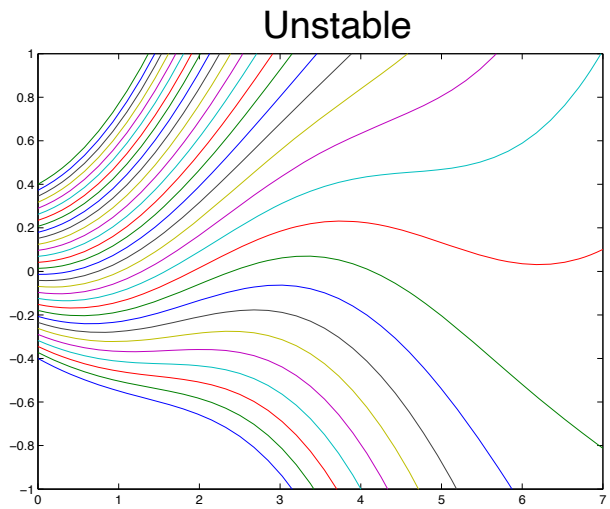
Runge-Kutta methods are more popularly used, because the change of the step size is trivial. In the procedure, step i only depends on step $i-1$ and the step size.

More efficient "multistep" algorithms can be done by changing step i depending on several previous steps. Commonly used in molecular dynamics and game physics.

Stability Analysis







A solution of an ordinary differential equation is called

- Stable: if the solutions of the initial-value problem with small changes on the initial value stay close to the original solution.
- Asymptotic stable: if it's stable and the solutions from small changes always converge to the original solution.
- Unstable: if the solutions from small changes diverge from the original solution.

Stability analysis

- Even for a stable solution, a numerical ODE solver can become unstable, if the step size is chosen too large.
- Stiff systems where different phenomena occur on different time scales require other solvers.....
- This is out of scope for this course, but you can learn more in e.g. Course 02686 & 02687 (in total 10 ECTS only on numerical methods for ODE's and PDE's)

Next week

In Chapter 7.4, we consider the ODE systems. A single differential equation

$$\frac{d\,x(t)}{dt} = f\big(t, x(t)\big)$$

is extended to a system of differntial equations

$$\frac{d\,\boldsymbol{x}(t)}{dt} = \boldsymbol{f}\big(t, \boldsymbol{x}(t)\big).$$

Instead of solving a scalar x, now we need solve a vector $\boldsymbol{x}$, and f is replaced by a vector function $\boldsymbol{f}$ in the same dimension as $\boldsymbol{x}$. The algorithms are similar, but now scalars are replaced by vectors.

So Chapter 7.4 can be quickly gone through. After that, we will deal with boundary-value problems, i.e. Chapter 11.1, and here we need both interpolation and equation solvers.