

Ordinary differential equations (ODE's). Initial Value Problem

$$y'(x) = f(x, y) \quad y(x_0) = a; \quad x \geq x_0$$

where $x \in \mathbb{R}$ and $y(x)$ is an N -dimensional function. The N -dimensional vector a is called the *Initial Condition*.

We can write this coordinate wise as

$$\begin{aligned} [y]_0'(x) &= f_0(x, [y]_0, \dots, [y]_{N-1}) & [y]_0(x_0) &= a_0 \\ [y]_1'(x) &= f_1(x, [y]_0, \dots, [y]_{N-1}) & [y]_1(x_0) &= a_1 \\ &\dots & & \\ [y]_{N-1}'(x) &= f_{N-1}(x, [y]_0, \dots, [y]_{N-1}) & [y]_{N-1}(x_0) &= a_{N-1} \end{aligned}$$

What a numerical solution will generate:

Notation: $[y]_n$ is the n 'th coordinate of vector y , and y_n is the numerical approximation of $y(x_n)$ obtained after n steps of the numerical integration method (NR uses the same notation for these !!!).

In numerical solutions to ordinary differential equations, we first define a stepsize h and

$$\begin{aligned} x_n &= x_0 + nh \quad n = 0, 1, 2, \dots \\ y_n &\simeq y(x_n) \quad n = 0, 1, 2, \dots \end{aligned}$$

where y_n is the numerical approximation to the true value $y(x_n)$.

$$y'(x) = f(x, y) \quad y(x_0) = a \quad x \geq x_0$$

where $x \in \mathbb{R}$ and $y(x)$ is an N -dimensional function. The N -dimensional vector a is called the *Initial Condition*.

Example:

$$\begin{aligned} u'(x) &= u(x) \cos(v(x)) & u(0) &= 1 \\ v'(x) &= -u(x)^3 & v(0) &= \frac{\pi}{2} \end{aligned}$$

$$\begin{aligned} N &= 2 \\ x_0 &= 0 \\ a &= \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} \equiv y_0 \\ y(x) &= \begin{pmatrix} [y]_0(x) \\ [y]_1(x) \end{pmatrix} \\ f(x, y) &= \begin{pmatrix} [y]_0(x) \cos([y]_1(x)) \\ -[y]_0(x)^3 \end{pmatrix} \end{aligned}$$

Higher order differential equations can also be written in this way:

Problems involving ordinary differential equations (ODEs) can always be reduced to the study of sets of first-order differential equations. For example the second-order equation

$$\frac{d^2 y}{dx^2} + q(x) \frac{dy}{dx} = r(x) \quad (17.0.1)$$

can be rewritten as two first-order equations,

$$\begin{aligned} \frac{dy}{dx} &= z(x) \\ \frac{dz}{dx} &= r(x) - q(x)z(x) \end{aligned} \quad (17.0.2)$$

In numerical solutions to ordinary differential equations, we first define a stepsize h and

$$\begin{aligned}x_n &= x_0 + nh & n = 0, 1, 2, \dots \\y_n &\simeq y(x_n) & n = 0, 1, 2, \dots\end{aligned}$$

where y_n is the numerical approximation to the true value $y(x_n)$.

$$y'(x) = f(x, y) \quad y(x_0) = a; \quad x \geq x_0$$

Explicit one-step methods (Runge-Kutta methods):

$$y_{n+1} = F(x_n, h, y_n, f)$$

(the function $F(x_n, h, y_n, f)$ is often computed with some set of sequential substeps).

We will often write this as

$$y_{n+1} = F(x_n, h, y_n, f) + \mathcal{O}(h^{k+1})$$

where the last term indicates that if we would have $y_n \equiv y(x_n)$, then we would get $\|y_{n+1} - y(x_{n+1})\| = \mathcal{O}(h^{k+1})$, where k is called the *order* of the numerical method.

1st order Runge-Kutta (Euler):

$$y_{n+1} = y_n + hf(x_n, y_n) + \mathcal{O}(h^2)$$

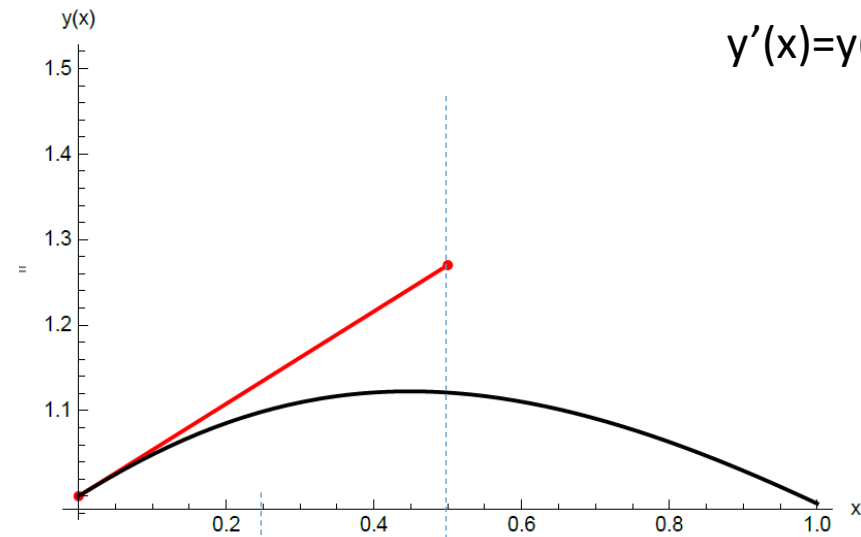
2nd order Runge-Kutta (Midpoint):

$$\begin{aligned}k_1 &= hf(x_n, y_n) \\k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) \\y_{n+1} &= y_n + k_2 + \mathcal{O}(h^3)\end{aligned}$$

$$y'(x) = f(x, y) \quad y(x_0) = a; \quad x \geq x_0$$

One step with 1st order Runge-Kutta (Euler).
Stepsize: $h=0.5$

$$y_{n+1} = y_n + h \boxed{f(x_n, y_n)} + O(h^2)$$



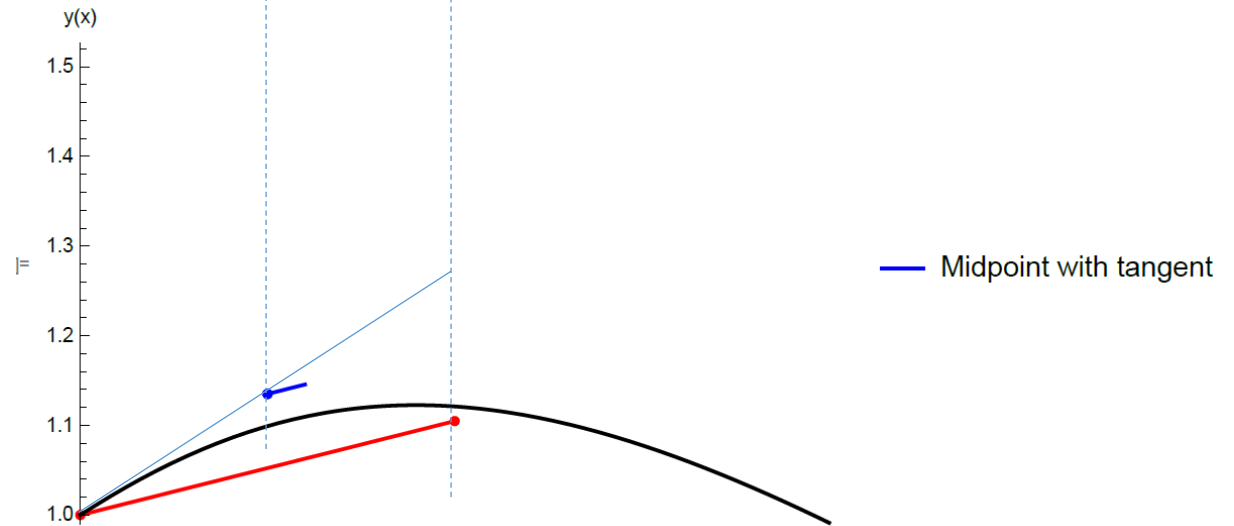
$$y'(x) = y(x) \cos(x + y(x)); \quad y(0) = 1$$

One step with 2nd order Runge-Kutta (Midpoint).
Stepsize: $h=0.5$

$$k_1 = h \boxed{f(x_n, y_n)}$$

$$k_2 = h \boxed{f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right)}$$

$$y_{n+1} = y_n + k_2 + O(h^3)$$



4th order Runge-Kutta:

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1)$$

$$k_3 = hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2)$$

$$k_4 = hf(x_n + h, y_n + k_3)$$

$$y_{n+1} = y_n + \frac{1}{6}k_1 + \frac{1}{3}k_2 + \frac{1}{3}k_3 + \frac{1}{6}k_4 + O(h^5)$$

Function evaluations:

As usual, we assume that the computationally expensive part is the computation of the function $f(x,y)$. For 1st order Runge-Kutta, we have one function evaluation per step. For 2nd order Runge-Kutta, it is two function evaluations and for 4th order Runge-Kutta, it is four function evaluations. Of course, we also seem to get higher accuracy. Our aim is to find the **most suitable method that gives the proven accuracy we want with as few function evaluations as possible.**

Example

$$\begin{aligned}u'(x) &= u(x) \cos(v(x)) & u(0) &= 1 \\v'(x) &= -u(x)^3 & v(0) &= \frac{\pi}{2}\end{aligned}$$

Defines the application.

In your code: Separate the application from the method !!!

$$\begin{aligned}N &= 2 \\x_0 &= 0 \\a &= \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} \equiv y_0 \\y(x) &= \begin{pmatrix} [y]_0(x) \\ [y]_1(x) \end{pmatrix} \\f(x, y) &= \begin{pmatrix} [y]_0(x) \cos([y]_1(x)) \\ -[y]_0(x)^3 \end{pmatrix}\end{aligned}$$

1st order Runge-Kutta (Euler):

$$y_{n+1} = y_n + hf(x_n, y_n) + O(h^2)$$

We can now perform one step with Euler with stepsize h to obtain

$$\begin{aligned}f(x_0, y_0) &= \begin{pmatrix} 0 \\ -1 \end{pmatrix} \\y_1 &= y_0 + hf(x_0, y_0) = \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} + h \begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{\pi}{2} - h \end{pmatrix}\end{aligned}$$

$$\begin{aligned} u'(x) &= u(x) \cos(v(x)) & u(0) &= 1 \\ v'(x) &= -u(x)^3 & v(0) &= \frac{\pi}{2} \end{aligned}$$

2nd order Runge-Kutta (Midpoint):

$$\begin{aligned} k_1 &= hf(x_n, y_n) \\ k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) \\ y_{n+1} &= y_n + k_2 + O(h^3) \end{aligned}$$

If we do one step with the midpoint method (2nd order Runge-Kutta), we get

$$\begin{aligned} f(x_0, y_0) &= \begin{pmatrix} 0 \\ -1 \end{pmatrix} \\ k_1 &= hf(x_0, y_0) = h \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \\ y_0 + \frac{1}{2}k_1 &= \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} + \frac{h}{2} \begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{\pi}{2} - \frac{h}{2} \end{pmatrix} \\ k_2 &= hf\left(x_0 + \frac{h}{2}, y_0 + \frac{1}{2}k_1\right) = h \begin{pmatrix} \cos\left(\frac{\pi}{2} - \frac{h}{2}\right) \\ -1 \end{pmatrix} \\ y_1 &= y_0 + k_2 = \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} + h \begin{pmatrix} \cos\left(\frac{\pi}{2} - \frac{h}{2}\right) \\ -1 \end{pmatrix} = \begin{pmatrix} 1 + h \cos\left(\frac{\pi}{2} - \frac{h}{2}\right) \\ \frac{\pi}{2} - h \end{pmatrix} \end{aligned}$$

$$\begin{aligned} N &= 2 \\ x_0 &= 0 \\ a &= \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} \equiv y_0 \\ y(x) &= \begin{pmatrix} [y]_0(x) \\ [y]_1(x) \end{pmatrix} \\ f(x, y) &= \begin{pmatrix} [y]_0(x) \cos([y]_1(x)) \\ -[y]_0(x)^3 \end{pmatrix} \end{aligned}$$

Order of a numerical method (global order):

$$y_{n+1} = F(x_n, h, y_n, f) + \mathcal{O}(h^{k+1})$$

where the last term indicates that if we would have $y_n \equiv y(x_n)$, then we would get $\|y_{n+1} - y(x_{n+1})\| = \mathcal{O}(h^{k+1})$, where k is called the *order* of the numerical method.

In applications, we will not be interested in the error after one step, but the error at some fixed x . If we use a a number of subdivisions

$$x_n = x_0 + nh \quad n = 0, \dots, M$$

so that $x = Mh$, we get a first approximation of the error at x as

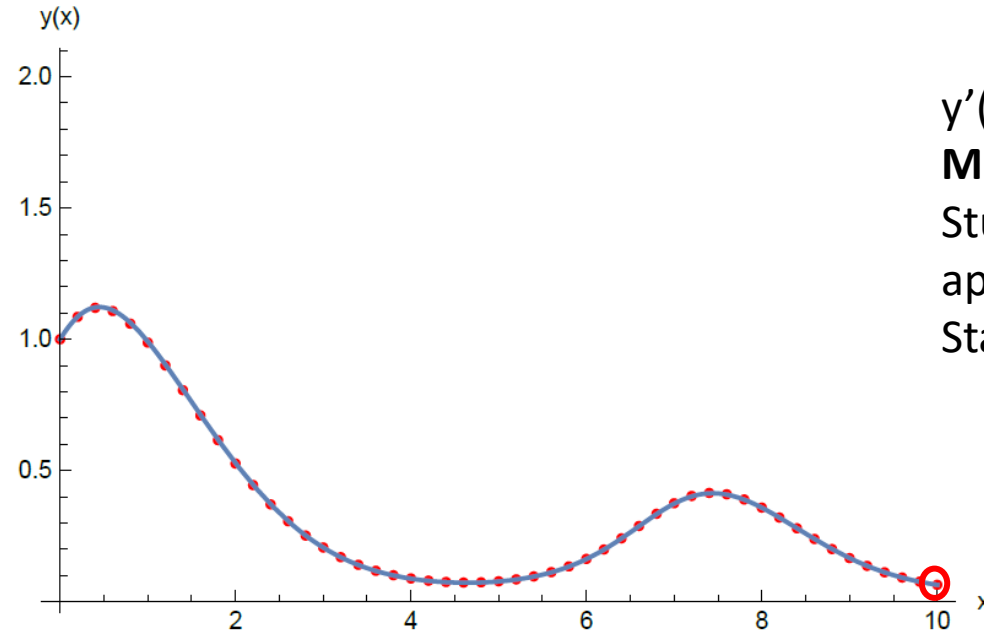
$$\|y_M - y(x)\| \simeq M * \mathcal{O}(h^{k+1})$$

Since $M = \frac{x}{h}$, we expect to get

$$\|y_M - y(x)\| \simeq \mathcal{O}(h^k)$$

which is why k (and not $k + 1$) is called the order of the method.

The term for one step $\mathcal{O}(h^{k+1})$ is called the "local order" of the method



$$y'(x) = y(x) \cos(x + y(x)); y(0) = 1$$

Midpoint method.

Studying the error on the numerical approximation to $y(10)$.

Start with $h=1$. Then $h=0.5$; 0.25 ;...

i	A(h _i)	A(h _{i-1}) - A(h _i)	Rich - alp ^k	A(h _i) - A	Rich-error	f-computations
1.	0.0569798	*	*	-0.00736924	*	20.
2.	0.0665769	-0.00959713	*	0.00222789	*	60.
3.	0.0649463	0.0016306	-5.88566	0.000597297	0.000543532	140.
4.	0.0644924	0.000453938	3.59211	0.000143359	0.000151313	300.
5.	0.0643838	0.000108616	4.17929	0.0000347431	0.0000362054	620.
6.	0.0643576	0.0000261993	4.14576	8.54381×10^{-6}	8.73311×10^{-6}	1260.

Implicit one-step methods:

$$y_{n+1} = F(x, h, y_n, y_{n+1}, f)$$

Here only the Trapezoidal method:

$$y_{n+1} = y_n + \frac{h}{2} (f(x_n, y_n) + f(x_{n+1}, y_{n+1})) + \mathcal{O}(h^3)$$

Perform an Euler step

$$y_{n+1}^* = y_n + hf(x_n, y_n)$$

Then use Newtons method to solve the system of potentially non-linear equations

Implementation:

$$\phi(y) = y - y_n - \frac{h}{2} (f(x_n, y_n) + f(x_{n+1}, y)) = 0$$

using $y = y_{n+1}^*$ as the initial guess and choose then $y_{n+1} = y$. One or at most two iterations will usually do to obtain an error that is negligible compared to the discretization error. For Newtons method, we obtain the Jacobian

$$J(y) = I - \frac{h}{2} J_f(y)$$

where J_f is the Jacobian wrt. y of $f(x_{n+1}, y)$.

$$\begin{aligned} u'(x) &= u(x) \cos(3x + v(x)) & u(0) &= 1 \\ v'(x) &= x^2 - u(x)^3 & v(0) &= \frac{\pi}{2} \end{aligned}$$

$$y_{n+1} = y_n + \frac{h}{2} (f(x_n, y_n) + f(x_{n+1}, y_{n+1})) + \mathcal{O}(h^3)$$

We obtained with Euler's method

$$\begin{aligned} f(x_0, y_0) &= \begin{pmatrix} 0 \\ -1 \end{pmatrix} \\ y_1 &= \begin{pmatrix} 1 \\ \frac{\pi}{2} - h \end{pmatrix} \end{aligned}$$

$$\phi(y) = \begin{pmatrix} [y]_0 \\ [y]_1 \end{pmatrix} - \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} - \frac{h}{2} \left[\begin{pmatrix} 0 \\ -1 \end{pmatrix} + \begin{pmatrix} [y]_0 \cos(3h + [y]_1) \\ h^2 - [y]_0^3 \end{pmatrix} \right]$$

$$J(y) = \begin{pmatrix} 1 - \frac{h}{2} \cos(3h + [y]_1) & \frac{h}{2} [y]_0 \sin(3h + [y]_1) \\ \frac{h}{2} 3[y]_0^2 & 1 \end{pmatrix}$$

We are then ready to use $y = y_1$ as the initial guess for solving $\phi(y) = 0$ with Newtons method.

Perform an Euler step

$$y_{n+1}^* = y_n + h f(x_n, y_n)$$

Then use Newtons method to solve the system of potentially non-linear equations

$$\phi(y) = y - y_n - \frac{h}{2} (f(x_n, y_n) + f(x_{n+1}, y)) = 0$$

using $y = y_{n+1}^*$ as the initial guess and choose then $y_{n+1} = y$. One or at most two iterations will usually do to obtain an error that is negligible compared to the discretization error. For Newtons method, we obtain the Jacobian

$$J(y) = I - \frac{h}{2} J_f(y)$$

where J_f is the Jacobian wrt. y of $f(x_{n+1}, y)$.

$$N = 2$$

$$x_0 = 0$$

$$a = \begin{pmatrix} 1 \\ \frac{\pi}{2} \end{pmatrix} \equiv y_0$$

$$y(x) = \begin{pmatrix} [y]_0(x) \\ [y]_1(x) \end{pmatrix}$$

$$f(x, y) = \begin{pmatrix} [y]_0(x) \cos(3x + [y]_1(x)) \\ x^2 - [y]_0(x)^3 \end{pmatrix}$$

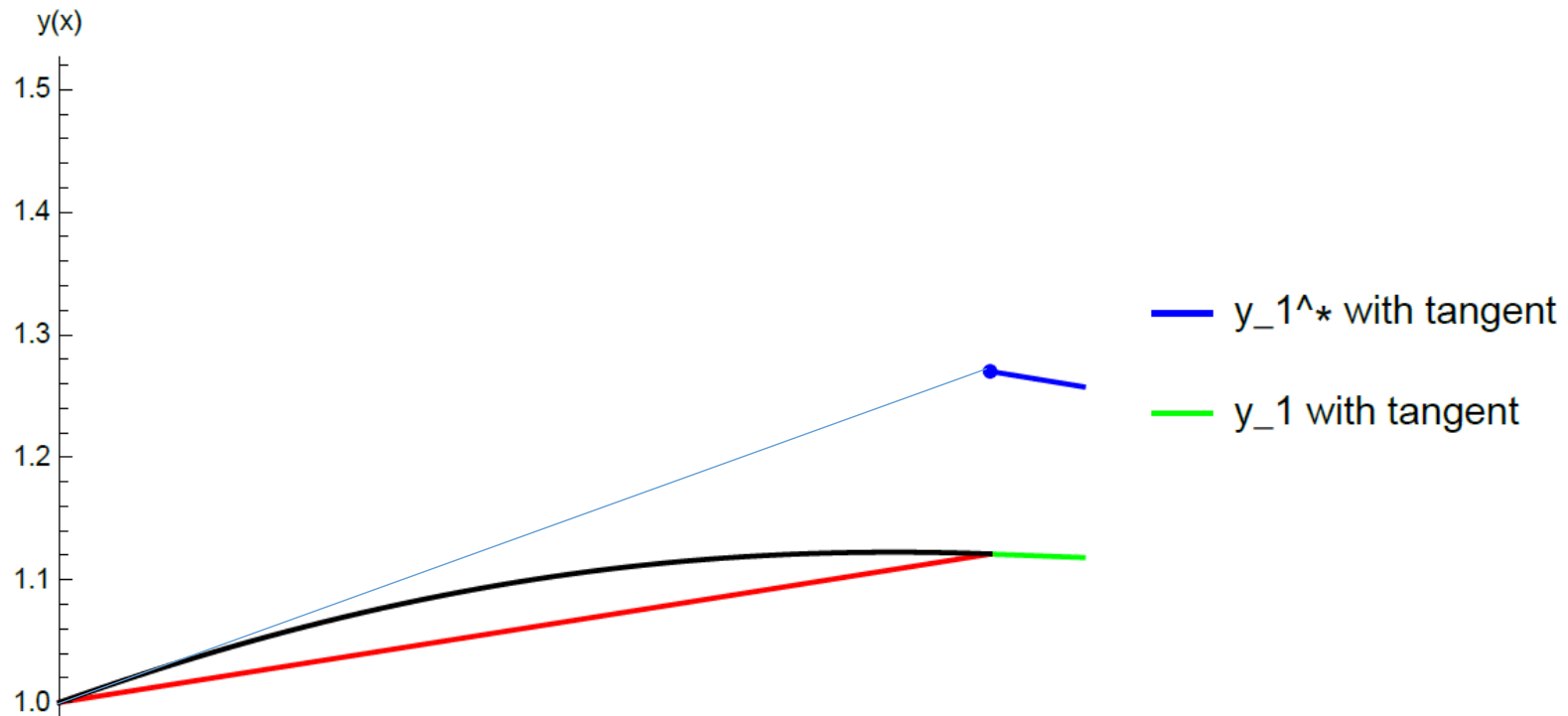
$$\phi(y) = y - y_n - \frac{h}{2} (f(x_n, y_n) + f(x_{n+1}, y))$$

$$J(y) = \begin{pmatrix} 1 - \frac{h}{2} \cos(3x + [y]_1) & \frac{h}{2} [y]_0 \sin(3x + [y]_1) \\ \frac{h}{2} 3[y]_0^2 & 1 \end{pmatrix}$$

$$y'(x) = y(x) \cos(x + y(x)); y(0) = 1$$

Trapezoidal method.

$$y_{n+1} = y_n + \frac{h}{2} (f(x_n, y_n) + f(x_{n+1}, y_{n+1})) + \mathcal{O}(h^3)$$



Two-step Leap-frog method:

$$y_{n+1} = y_{n-1} + 2hf(x_n, y_n) + \mathcal{O}(h^3)$$

Do an Euler step first to initiate the method with y_0 and y_1 .

Exercise:

$$\begin{aligned} u'(x) &= u(x)v(x) & u(0) &= 1 \\ v'(x) &= -u(x)^2 & v(0) &= 1 \end{aligned}$$

Solve with Euler, Midpoint, Trapezoidal, Leap-frog and 4th order Runge-Kutta

Consider $x=10$ and estimate the order using Richardson

Subdivide h with 2 until you reach an accuracy on $u(x)$ of 10^{-6}

Establish a table like on slide 9 (of course without the $A(h)$ - A column)

Table from slide 9:

i	A(h _i)	A(h _{i-1}) - A(h _i)	Rich-alp ^k	A(h _i) - A	Rich-fejl	Antal f-ber.
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