Lecture Notes 5/9 - 2023 - Ordinary differential equations (1)

ODEs can be used to describe many physical, biological or chemical systems.

Examples: radioactive decay, population dynamics, concentration of a certain compound in a lake or tank, mechanical problems.

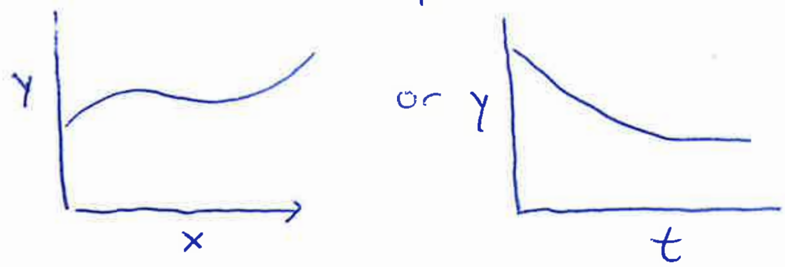
The equations are derived using certain laws and assumptions

The theory we will go through is mostly taken from Chapter 7 in Jan Kiusalaas book: Numerical Methods in Engineering with Python3 page 246-263.

We will focus on differential equations of first order: $y' = f(x,y)$. Note y' can also be written as $\frac{dy}{dx}$

Sometimes the notation $\dot{y}$ is also used. In this case $\dot{y} = \frac{dy}{dt}$, t is time

From the differential equation, we want to find the function $y(x)$ that shows how y varies as function of x.



if $y(t)$ t is time

But to find $y(x)$ we need to solve the differential equation. In some cases we can find exact solutions. But ~~is~~ often we need to use a numerical method to approximate the solution.

Here we will concentrate on two methods

1) Euler method
2) 4th order Runge Kutta method

Simple example:

$$y' = 0$$

$$\frac{dy}{dx} = 0$$

$\int y' = \int 0$ We integrate and get an integration constant c.

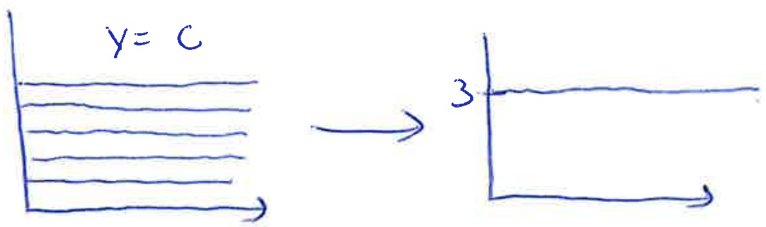
$y(x) = c$ So all functions $y(x) = c$ are solutions to this

Therefore in order to pick out a unique solution we need an auxiliary condition $y(a) = \alpha$

So if we specify

$y' = 0$ & $y(0) = 3$ we have what we call an initial value problem. The extra information $y(0) = 3$ makes it possible to determine the integration constant C.

$y = 3$ will be the unique solution



Order of differential equation:

If there is only a first derivative in the differential equation: $y' = f(x, y)$ $y(0) = \alpha$ we have a first order diff equation.

However there can be higher order derivatives involved.

e.g $y'' + y' - 6y = 0$ or $y'' = -y' + 6y$. This is an example of a second order linear differential equation

In this case we need to specify two extra conditions to determine the two integration constants that will occur when solving the equation

$$y'' + y' - 6y = 0 \ \& \ y(0) = C_1, y'(0) = C_2$$

But note that we can rewrite a second order or higher differential equation as a system of first order differential equations. This will be shown later.

Linear vs Nonlinear equations:

The ordinary differential equation is classified as liner if the equation is a linear combination of the derivatives involved:

$$a_0(x)y^{(n)} + a_1(x)y^{(n-1)} + \quad + a_n(x)y = g(x)$$

Examples of linear ordinary diff equations

1) $y'' + y' - 6y = 0$
2) $xy' + 2y = 4x^2$, $y(1) = 2$
3) $y' + 4y = x^2$, $y(0) = 1$ (page 250 in book)

Example of nonlinear equations:

$y' = y^{1/3}$, $y(0) = 0$

$y' = (1 - x^2 - y^2)^{1/2}$

The mathematical theory & analytical techniques for solving linear differential equations are highly developed. But for nonlinear equations it is not that satisfactory.

So for more difficult problems we need to use numerical methods to produce solutions.

Here we will study

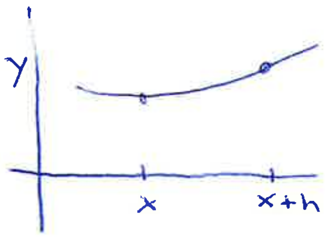
1) The first order Euler method
2) 4th order Runge Kutta method.

Euler method:

We derive this from truncating the Taylor Polynomial formula

The Taylor formula:

$$y(x+h) = y(x) + y'(x)\cdot h + \frac{y''(x)\cdot h^2}{2!} + \frac{y'''(x)\cdot h^3}{3!} + + = \sum_{k=0}^{\infty} \frac{y^{(k)}(x)\cdot h^k}{k!}$$



It states that we can find $y(x+h)$ if we know all the derivatives in x.

If we now neglect the ~~terms~~ terms after $y'(x)\cdot h$ we can approximate

$$y(x+h) \approx y(x) + y'(x)\cdot h$$

The error/deviation will then be: $E = \frac{1}{2} y''(x) h^2 = O(h^2)$

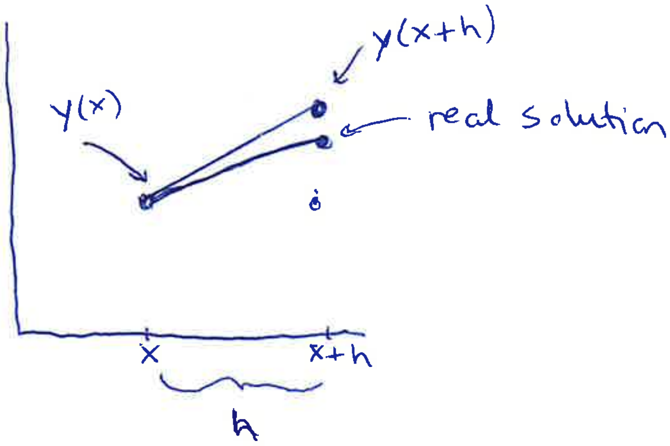
The most dominating term that we truncated is this one.

The differential equation is $y' = f(x,y)$. This is now inserted into the truncated expression

$$y(x+h) = y(x) + f(x,y)\cdot h.$$

So if we know the values in point x (right hand side), we can predict the value $y(x+h)$. h will be the step between the discrete points.

From $y(x+h) = y(x) + y'(x)\cdot h$ we can see that we approximate forward with a tangent. Since $y'(x)$ is the slope:



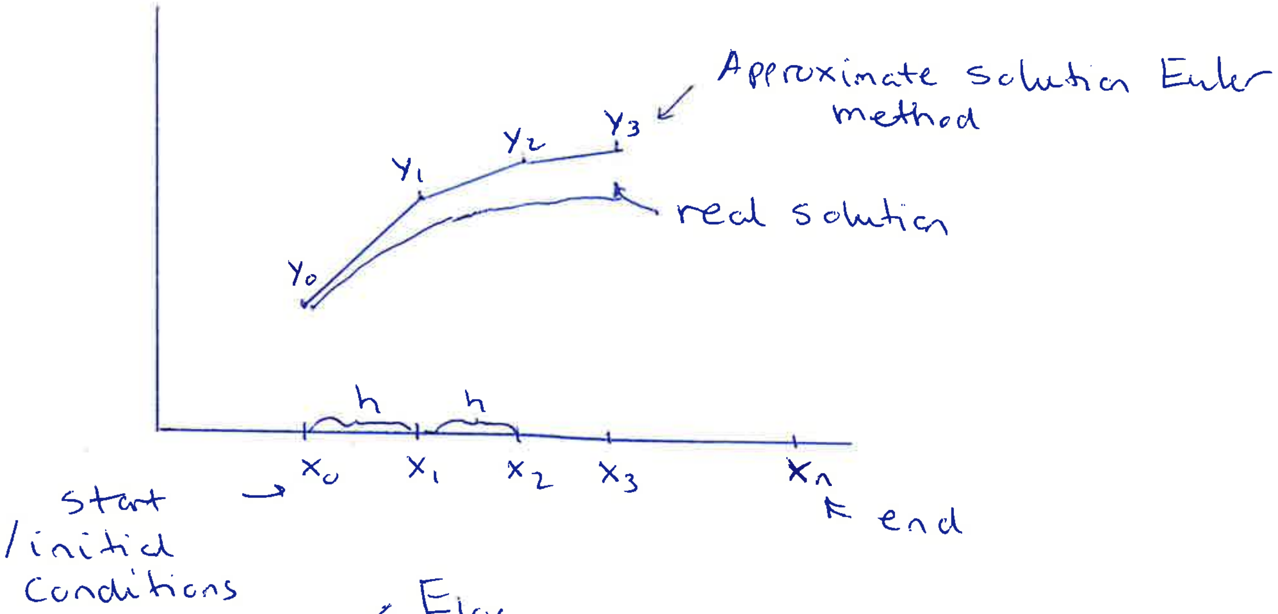
So to summarise:

$y' = f(x,y)$, $y(x_0) = y_0$ Our differential equation with initial conditions

We discretize and choose size of step h

Euler method: $y_{k+1} = y_k + h \cdot f(x_k, y_k)$, $k = 0, 1, 2, \ldots, n-1$

new value is calculated based on known old values where we start with that we know x_0, y_0 from the initial conditions.



The local error / E_{loc} caused by the truncation of the Taylor polynoma was seen to be $O(h^2)$ for each step.

Total number of step are: $\frac{x_n - x_0}{h}$

So the accumulated error will be of the order:

$$E_{acc} = \frac{x_n - x_0}{h} \cdot E_{loc} = \frac{x_n - x_0}{h} \cdot h^2 = O(h)$$

So this is a first order method (h to the power of 1)

If it was $O(h^2)$ or $O(h^4)$, the method would be second or fourth order.

The higher order, the more accurate.

So Euler method is only first order and not very accurate.

We need to use very small step size h to get close to the real solution

So by letting h get smaller and smaller, the approximate numerical solution provided by the Euler method will get closer and closer to the real solution. We say that the numerical solution converges to the real solution

But a first order method will converge slower than a higher order method. We need to reduce the step more and this will come at the price of increased computer costs/time consume.

We will now look at Example 7.1 page 250 in the book of J. Kiusalaas.

We have the initial value problem

$$y' + 4y = x^2, \quad y(0) = 1$$

We can rewrite this as $y' = f(x,y)$ where $f(x,y) = x^2 - 4y$

It can be shown by using the method with integrating factor that the exact solution becomes:

$$y(x) = \frac{31}{32} e^{-4x} + \frac{1}{4}x^2 - \frac{1}{8}x + \frac{1}{32}$$

Download the JupyterNotebook: Eulermethod Example 1

We will study how the Euler method is implemented when we simulate from $x = 0$ to $x = 0.03$ with steps $h = 0.01$.

We will study the errors by comparing with the exact solution + we will change simulation time to 0.5 s and see the difference between using $h = 0.01$ and $h = 0.1$

Second example: Radioactive decay.

The radioactive isotope Thorium 234 disintegrates at a rate proportional to the amount present. 100mg of this material is reduced to 82.04mg in one week. Let $Q(t)$ be the amount of Thorium 234 present at any time. Q is in milligrams and t is in days.

Why can we argue that Q must satisfy the following differential equation?

$$\frac{dQ}{dt} = -rQ$$

Answer: This is because the disintegration/reduction in amount of Thorium must be proportional to the amount of Thorium present. $\frac{dQ}{dt}$ is proportional to Q and r is the proportionality constant. There must be a minus since we have a reduction of Q. $\frac{dQ}{dt}$ is negative.

We will now derive the exact solution to this equation/problem + find the half life isotope (halveringstiden).

Then we will afterwards see how the problem can be solved by simulation using Euler method.

We want the exact solution just for comparison.

In many cases, we dont have exact solutions.

Analytical solution:

This problem must be solved using the method of separation of variables.

$$\frac{d\varphi}{dt} = -r\varphi$$

$\varphi(0) = 100\,mg$

+ we know that we have 82.04 mg after one week.

t is in days

$$\downarrow$$

$$\frac{d\varphi}{\varphi} = -r\,dt$$

$$\downarrow$$

$$\int \frac{d\varphi}{\varphi} = -\int r\,dt$$

$$\downarrow$$

$$\ln\varphi = -rt + C_1$$

$$\downarrow$$

named C

$$e^{\ln\varphi} = e^{-rt + C_1} = e^{-rt} \cdot e^{C_1}$$

$$\downarrow$$

$$\varphi(t) = C e^{-rt}$$

We now determine C_1 ~~us~~ and r using the extra information.

$$\varphi(0) = 100\,mg = C \cdot e^{-r \cdot 0}$$

$$100\,mg = C\, e^{0} \rightarrow 1$$

$$C = 100\,mg$$

To find r we use that 100 mg is reduced to 82.04 mg in 7 days

$$\varphi(t) = 100\, e^{-rt}$$

$$82.04 = 100 \cdot e^{-r7}$$

logaritmic rule

$$e^{-7r} = \cancel{100}\ \frac{82.04}{100} = 0{,}8204$$

$$\ln(e^{-7r}) = \ln(0.8204)$$

$$-7r \underbrace{\ln e}_{1} = \ln(0.8204)$$

$$r = -\frac{\ln(0.8204)}{7} = +0{,}02828\ \text{day}^{-1}$$

$$\varphi(t) = 100\, e^{-0{,}02828t},$$

t in days

φ in mg

Half life / Halveringstid for the isotope:

We start with 100 mg. First half is when we have 50 mg. Find out ~~what~~ how long time it takes.

$$\varphi(t) = 100 e^{-0{,}02828t}$$

$$50 = 100 e^{-0{,}02828t}$$

$$e^{-0{,}02828t} = 0{,}5$$

$$\ln(e^{-0{,}02828t}) = \ln(0.5)$$

$$-0{,}02828t \ln e = \ln(0.5)$$

$$t = \frac{\ln 0{,}5}{-0{,}02828} = \underline{\underline{24{,}51\ \text{days}}}$$

This is the half life.

Numerical Solution / Euler Method

$$\frac{d\varphi}{dt} = -r\varphi, \quad \varphi(0) = 100\,\text{mg}, \quad r = 0{,}02828\ \text{day}^{-1}$$

Here we discretize in time using a timestep size Δt

$$\varphi_{k+1} = \varphi_k + \Delta t * (-r\varphi_k), \quad k = 0, 1, 2, 3 \text{ etc}$$

We will simulate for 50 days and compare the exact solution and numerical solution for various Δt.
We will start with $\Delta t = 5$ days and then reduce timestep until we think that the numerical solution has converged to the exact solution.

Also estimate the half life from the simulation

$\boxed{\text{Download: Eulermethod\_Example2}}$

Runge Kutta 4th order method

We recall that the Euler method was of order $O(h)$. First order. However, there is more accurate methods available. The higher order the more accurate

Both the second order Runge Kutta and the fourth order method are also derived from the Taylor Polynomial formula

$$y(x+h) = y(x) + y'(x)\cdot h + \frac{y''(x)\cdot h^2}{2!} + \frac{y'''(x)\cdot h^3}{3!} + \cdots = \sum_{k=0}^{\infty} \frac{y^{(k)}(x)\cdot h^k}{k!}$$

The idea of these higher order methods is to use more terms on the right hand side of the equation above. We include more terms.

We will not go into details but just present and implement the fourth order Runge Kutta method.

$y' = f(x,y)$ $\quad y(x_0) = y_0$, h is step size

$$K_0 = h\cdot f(x,y)$$
$$K_1 = h\, f\left(x+\frac{h}{2}, y+\frac{K_0}{2}\right)$$
$$K_2 = h\, f\left(x+\frac{h}{2}, y+\frac{K_1}{2}\right)$$
$$K_3 = h\, f(x+h, y+K_2)$$

Page 255 in book

$$y(x+h) = y(x) + \frac{1}{6}(K_0 + 2K_1 + 2K_2 + K_3)$$

Download RungeKutta_and_EulerMethodExample3

We are back to the problem
$y' = f(x,y)$ where $f(x,y) = x^2 - 4y$, $y(0) = 1$

1) Check if the implementation of the fourth order Runge Kutta method seems correct?
2) Let Xend=1, Vary h, h=0,5, h=0,2, h=0,1, h=0.05, h=0.01
Which method converges fastest towards the exact solution? What should the h be for Eulermethod VS 4th order Runge Kutta?
3) Reflect upon: How should one know what h should be if we dont have an exact solution to compare with?

Download RungeKutta_and_EulerMethod_Example4

We are back to the problem Radioactive decay
$\frac{d\varphi}{dt} = -r\varphi$, $\varphi(0) = 100$ mg, $r = 0{,}02828\ \text{day}^{-1}$
t is in days
We simulate 100 days. $\Delta t = 25$ days initially.
Reduce timestep and try to answer the following:
1) What timestep do you recommend for the 4th order Runge Kutta method?
2) What timestep do you recommend for Euler method

(Keep in mind that we can of course choose very small timesteps but computing time but also round off errors in the machine must be kept in mind. So stop reduction when it seems good enough)