Excercise 5

Short Intro

Derivatives

Definition

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

We can find approximate values for dervivatives of some function by using Taylor-series:

$$f(x) = \sum_{i=0}^{\infty} \frac{f^{(i)}(x_0)}{i!} (x - x_0)^i$$

• 1st derivative

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{1}{6}f'''(x_i)h^2 + \dots$$
(1)

• 2nd derivative

$$f''(x_i) = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} - \frac{1}{12}f^{(4)}(x_i)h^2 - \dots$$
(2)

• 3rd derivative

$$f'''(x_i) = \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2h^2} - \frac{1}{4}f^{(5)}(x_i)h^2 + \dots$$
(3)

- If we want calculate derivatives at the end points of the data $f'(x_1)$ and $f'(x_n)$, we must set some boundary conditions eg. $f(x_1-h) = f(x_n+h) = 0$.
- Note: You can also define interpolating function and derivate it.

Integration

• Definite Integral of some fuctions is defined as limit of Riemann sum

$$\int_{a}^{b} f(x)dx = \sum_{i=1}^{n-1} f(t_i)(x_{i+1} - x_i)$$

where step $[x_i, x_{i+1}]$ gets smaller. Boundaries: $x_1 = a, x_n = b$

• Let $x_{i+1} - x_i = h$, i = 1, ..., n-1 and $f(x_i) \equiv f_i$. By setting $t_i = x_i$, we get simple approximation

$$\int_{x_1}^{x_n} f(x) \, dx \approx h \sum_{i=1}^{n-1} f_i$$

- Better approximations could be made by interpolating data with piecewise defined function.
 - If q_i are 1st order polynomia, $q_i(x) = a_i(x x_i) + b_i$, we get so called *Trapezoidal rule*:

$$\int_{x_1}^{x_n} f(x) \, dx \approx h \sum_{i=1}^{n-1} \frac{f_i + f_{i+1}}{2} = \frac{f_1}{2} + \sum_{i=2}^{n-1} f_i + \frac{f_n}{2}$$

ex.

- 1. Read Sections 1.5.2-3 ja 1.6.2. and familiarise yourself with functions D, Dt, Integrate ja NIntegrate.
- 2. Let $f(x) = \sin \frac{1}{x}$. Make (again) a table of data points $(x_i, f(x_i))$ when $a \le x_i \le 2, i = 1, ..., n, a = 0.5 ... 0.01$ and n = 10 ... 50. (You can choose values freely).

Calculate 1st order approximations of $f'(x_i)$ and $f''(x_i)$ with formulas derived from Taylor-series. Listplot original function and derivatives. Compare approximation with derivative calculated with build-in function.

3. Radioactive decay obeys differential equation:

$$\frac{dN(t)}{dt} = -\lambda N(t),$$

where N(t) is number of active nuclei at time t. λ is decay constant: $\lambda = (\ln 2)/T_{1/2}$ and $T_{1/2}$ is half-life. Let $\lambda = 0.1 \,\mathrm{s}^{-1}$ and $N(0) = 10^{25}$. Replace derivative dN/dt with approximation

$$N'(t_i) = \frac{N_{i+1} - N_i}{h}$$

and solve N_{i+1} as a function of $N_i - t_{i+1} - t_i = h$ and h can have values $h = 10^{-4} \dots 0.1$. In other words solve N at t_i , $i = 2, \dots, n$ $(N(t_1) = N(0))$ to some large n and plot it. Compare approximation with the excact solution $N(t) = N(0)e^{-\lambda t}$.

4. Object has acceleration g(t) which varies in time:

$$a(t) = \frac{d^2x(t)}{dt^2} = g(t),$$

from which

$$v(t) = \frac{dx(t)}{dt} = v(0) + \int_0^t a(t')dt',$$

$$x(t) = x(0) + \int_0^t v(t')dt'.$$

Let g(t) = ct, where $c = 0.1 \text{ ms}^{-3}$, and initial conditions x(0) = 0, $v(0) = 1 \text{ ms}^{-1}$. Let's denote $t_i = (i-1)h$, $i = 1, \ldots, n$ where h = 0.01 s. Calculate first the velocities $v(t_i)$ and then the location x of the object at time t_i . Use first the build-in function Integrate and then approximate integrals using trapezoidal rule.

and