Exercise 6

October 19, 2021

1 Exercises 6: Numerical Solution of ODE's 1

TMA4130 - Mathematics 4N / TMA4135 - Mathematics 4D

- Date: **Oct 6, 2021**
- Submission deadline: **Oct 20, 2021**

If you want to have a nicer theme for your jupyter notebook, download the cascade stylesheet file calculus4N.css and execute the next cell:

[71]:
```
from IPython.core.display import HTML
def css_styling():
    try:
        with open("calculus4N.css", "r") as f:
            styles = f.read()
            return HTML(styles)
    except FileNotFoundError:
        print("Not found")
        pass #Do nothing

# Comment out next line and execute this cell to restore the default notebook␣
↪style
css_styling()
```

[71]:
```
<IPython.core.display.HTML object>
```

[72]:
```
import matplotlib
matplotlib.rcParams.update({'font.size': 12})
import matplotlib.pyplot as plt
import numpy as np

plt.xkcd()
newparams = {'figure.figsize': (6.0, 6.0), 'axes.grid': True,
             'lines.markersize': 8, 'lines.linewidth': 2,
             'font.size': 14}
plt.rcParams.update(newparams)
```

In this exercise set you will be analyzing and implementing the following explicit Runge-Kutta methods:

Midpoint rule

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$$

Gottlieb & Gottlieb's 3-stage Runge-Kutta (SSPRK3)

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 \\ \hline & \frac{1}{6} & \frac{1}{6} & \frac{2}{3} \end{array}$$

1.0.1 Exercise 1

Convergence orders Calculate analytically the convergence order's of the two methods. Use the order's conditions given in the lectures.

[73]:
```
# creates a function that will return the convergene order given a vector b, n x␣
↪n matrice and a vector c
def calculate_convergence(a, b, c):
    n = len(b)
    if (sum(b) == 1):
        sum_order2 = 0
        for i in range(n):
            sum_order2 += b[i] * c[i]

        if (sum_order2 == 1/2):
            sum_order3_1 = 0
            sum_order3_2 = 0
            for i in range(n):
                sum_order3_1 += b[i] * c[i]**2
                for j in range(n):
                    sum_order3_2 += b[i] * a[i][j] * c[j]

            if (sum_order3_1 == 1/3 and sum_order3_2 == 1/6):
                sum_order4_1 = 0
                sum_order4_2 = 0
                sum_order4_3 = 0
                sum_order4_4 = 0

                for i in range(n):
                    sum_order4_1 += b[i] * c[i]**3
                    for j in range(n):
                        sum_order4_2 += b[i] * c[i] * a[i][j] * c[j]
                        sum_order4_3 += b[i] * a[i][j] * c[j]**2
                        for k in range(n):
                            sum_order4_4 += b[i] * a[i][j] * a[j][k] * c[k]
                if (sum_order4_1 == 1/4 and sum_order4_2 == 1/8 and sum_order4_3␣
↪== 1/12 and sum_order4_4 == 1/24):
```

```
                return 4
            else:
                return 3
        else:
            return 2
    else:
        return 1
else:
    return 0
```

[74]:
```
# midpoint rule
a_m = np.array([[0, 0], [1/2, 0]])
b_m = np.array([0, 1])
c_m = np.array([0, 1/2])

print("Order of convergence for midpoint rule:", calculate_convergence(a_m, b_m,␣
 ↪c_m))

# SSPRK3
a_ssp = np.array([[0, 0, 0], [1, 0, 0], [1/4, 1/4, 0]])
b_ssp = np.array([1/6, 1/6, 2/3])
c_ssp = np.array([0, 1, 1/2])

print("Order of convergence for SSPRK3:", calculate_convergence(a_ssp, b_ssp,␣
 ↪c_ssp))
```

```
Order of convergence for midpoint rule: 2
Order of convergence for SSPRK3: 3
```

1.0.2 Exercise 2

Implementing and testing the methods In this exercise we will numerically solve the ODE

$$y'(t) = f(y), \quad y(0) = y_0$$

in the interval $t \in [0, T]$.

a) Implement two Python functions `explicit_mid_point_rule` and `ssprk3` which implement the Runge-Kutta methods from Exercise 1. Each solver function should take as arguments: * The initial value y_0 * The inital time t_0 * The final time T * The right-hand side f * The maximum number of time-steps N_{max}

The function should return two arrays: * One array `ts` containing all the time-points $0 = t_0, t_1, ..., t_N = T$ * One array ys containing all the function values $y_0, y_1, ..., y_N$

Test the methods on the ODE

$$y'(t) = -y(t), \quad y(0) = 1, \quad t \in [0, 10].$$

Hint: Use the code for `explicit_euler` in the lecture notes or use the supporting material e.g. `Heun` in IntroductionNuMeODE, and modify it to each required method.

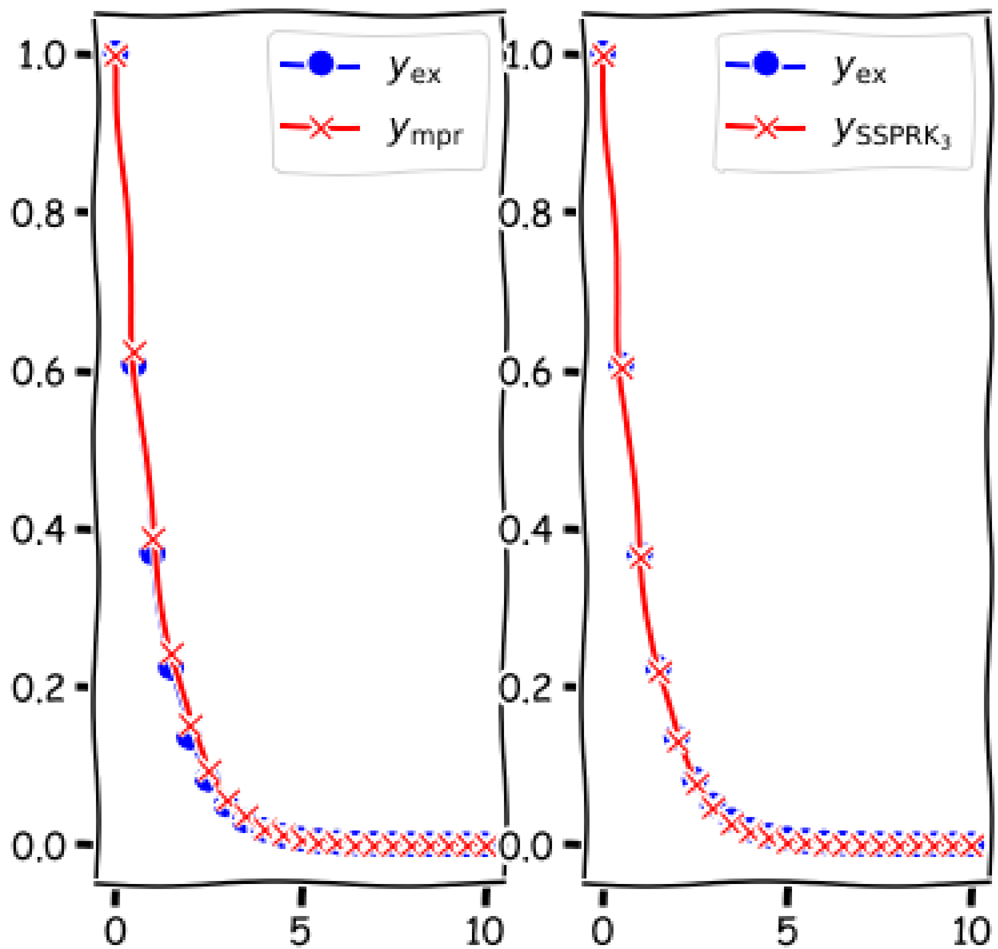
[75]:
```
def explicit_midpoint_rule(y0, t0, T, f, N_max):
    ts = [t0]
    ys = [y0]
    tau = (T - t0)/N_max

    # butcher table
    a = np.array([[0, 0], [1/2, 0]])
    b = np.array([0, 1])
    c = np.array([0, 1/2])

    s = len(b)
    ks = [np.zeros_like(y0, dtype=np.double) for s in range(s)]

    while (ts[-1] < T):
        t, y = ts[-1], ys[-1]
        # computing k_j's
        for j in range(s):
            dY = 0
            for l in range(j):
                dY += a[j][l] * ks[l]
            ks[j] = f(t + c[j] * tau, y + tau * dY)
        dY = 0
        for j in range(s):
            dY += b[j]*ks[j]
        ts.append(t + tau)
        ys.append(y + tau*dY)

    return ts, ys

def explicit_ssprk3(y0, t0, T, f, N_max):
    # initial values
    ts = [t0]
    ys = [y0]
    tau = (T - t0)/N_max

    # butcher table
    a = np.array([[0, 0, 0], [1, 0, 0], [1/4, 1/4, 0]])
    b = np.array([1/6, 1/6, 2/3])
    c = np.array([0, 1, 1/2])

    s = len(b)
    ks = [np.zeros_like(y0, dtype=np.double) for s in range(s)]

    while (ts[-1] < T):
```

```python
        t, y = ts[-1], ys[-1]
        # computing k_j's
        for j in range(s):
            dY = np.zeros_like(y, dtype=np.double)
            for l in range(j):
                dY += a[j][l] * ks[l]
            ks[j] = f(t + c[j] * tau, y + tau * dY)
        dY = np.zeros_like(y, dtype=np.double)
        for j in range(s):
            dY += b[j]*ks[j]
        ts.append(t + tau)
        ys.append(y + tau*dY)
    return np.array(ts), np.array(ys)
```

[76]:

```python
y0 = 1
t0 = 0
T = 10
N_max = 20



def f(t, y):
    return -y

# exact solution (exp(-t))
def y_ex(t):
    return np.exp(-t)

fig, axes = plt.subplots(1,2)
ts, ys_mdr = explicit_midpoint_rule(y0, t0, T, f, N_max)
ys_ex = []
for t in ts:
    ys_ex.append(y_ex(t))
axes[0].plot(ts, ys_ex, 'bo-')
axes[0].plot(ts, ys_mdr, 'rx-')
axes[0].legend(["$y_{\mathrm{ex}}$", "$y_{\mathrm{mpr}}$" ])
ts, ys_ssprk3 = explicit_ssprk3(y0, t0, T, f, N_max)
axes[1].plot(ts, ys_ex, 'bo-')
axes[1].plot(ts, ys_ssprk3, 'rx-')
axes[1].legend(["$y_{\mathrm{ex}}$", "$y_{\mathrm{SSPRK_3}}$" ])
```

[76]: <matplotlib.legend.Legend at 0x233bfef69c8>



b) We will now numerically investigate the RK-methods. We can do this since we know what the exact solution to the ODE above is. We assume that the error $e = |y(T) - y_N|$ when using step size τ is approximately

$$e \approx C\tau^p$$

for some $C > 0$ and p. Note that p is what we call the convergence order. We assume that p and C is the same when using different step sizes h. Let e_1 and e_2 be the errors when using step sizes h_1 and h_2. Then we have

$$\frac{e_1}{e_2} \approx \frac{\tau_1^p}{\tau_2^p} = \left(\frac{\tau_1}{\tau_2}\right)^p.$$

Taking logarithms on both sides we get

$$\log(e_1/e_2) \approx p \log(\tau_1/\tau_2)$$

or \$

$$p \approx \frac{\log(e_1/e_2)}{\log(\tau_1/\tau_2)}. \tag{1}$$

$ The value on the right-hand side of this equation is what we call the Experimental Order of Convergence, or EOC. We will now try to estimate the order of convergence using EOC-values.

Do the following for each method: 1. For m=0,...,5, set $\tau_m = 2^{-m}$ and find the value of N_{max} for each m. 2. Find the numerical solution $y_{N(m)}$ of the ODE at $T = 10$. 2. Calculate the error $e_m = |y(10) - y_{N_{max,m}}|$. 3. Calculate the EOC for neighbouring step sizes, that is using equation (1) above with e_m and e_{m+1} for $m = 0, ..., 4$. This should give you 5 different approximations.

Draw a conclusion about the order of convergence p for each method. Does it agree with the result in exercise 1?

[77]:
```
# N_max will be the same for both methods.
m = [i for i in range(6)]
t0 = 0
T = 10
N_maxes = []
# N_max = (T - t0)*2^m
for i in m:
    N_maxes.append((T - t0) * 2**i)

# solving the ODE with different N_max
# dont need to store the result, only need to store the last value, eg y_N
ys_Nmax_mpr = []
ys_Nmax_ssprk = []

for N_m in N_maxes:
    ts, ys = explicit_midpoint_rule(y0, t0, T, f, N_m) # f is the same as␣
 ↪defined above
    ys_Nmax_mpr.append(ys[-1])
    ts, ys = explicit_ssprk3(y0, t0, T, f, N_m)
    ys_Nmax_ssprk.append(ys[-1])

# calculating the errors
e_m_mpr_list = []
e_m_ssprk_list = []

for i in range(6):
    # midpoint rule
    e_m_mpr = np.absolute(y_ex(10) - ys_Nmax_mpr[i])
    e_m_mpr_list.append(e_m_mpr)
    # SSPRK3
    e_m_ssprk = np.absolute(y_ex(10) - ys_Nmax_ssprk[i])
    e_m_ssprk_list.append(e_m_ssprk)

# finally calculating the EOC
eoc_mpr_list = []
eoc_ssprk_list = []
```

```python
for i in range(5):
    # midpoint rule
    p_mpr_i = (np.log(e_m_mpr_list[i]/e_m_mpr_list[i+1]))/(np.log(2**(-i)/
 ↪2**(-i-1)))
    eoc_mpr_list.append(p_mpr_i)
    # SSPRK3
    p_ssprk_i = (np.log(e_m_ssprk_list[i]/e_m_ssprk_list[i+1]))/(np.log(2**(-i)/
 ↪2**(-i-1)))
    eoc_ssprk_list.append(p_ssprk_i)

print("Midpoint rule:")
for i in range(5):
    print(f"tau_{i} = {2**(-i)},tau_{i+1} = {2**(-i-1)} gives "
          + f"experimental order of convergence p = {eoc_mpr_list[i]}")

print("\nSSPRK3:")
for i in range(5):
    print(f"tau_{i} = {2**(-i)},tau_{i+1} = {2**(-i-1)} gives "
          + f"experimental order of convergence p = {eoc_ssprk_list[i]}")
```

```
Midpoint rule:
tau_0 = 1,tau_1 = 0.5 gives experimental order of convergence p =
4.641084409856239
tau_1 = 0.5,tau_2 = 0.25 gives experimental order of convergence p =
2.618767003133043
tau_2 = 0.25,tau_3 = 0.125 gives experimental order of convergence p =
2.2053567418841813
tau_3 = 0.125,tau_4 = 0.0625 gives experimental order of convergence p =
2.0834717759359433
tau_4 = 0.0625,tau_5 = 0.03125 gives experimental order of convergence p =
2.0375876961837682

SSPRK3:
tau_0 = 1,tau_1 = 0.5 gives experimental order of convergence p =
3.0609310003784023
tau_1 = 0.5,tau_2 = 0.25 gives experimental order of convergence p =
3.244464219011232
tau_2 = 0.25,tau_3 = 0.125 gives experimental order of convergence p =
3.1402030351845105
tau_3 = 0.125,tau_4 = 0.0625 gives experimental order of convergence p =
3.0717942133260796
tau_4 = 0.0625,tau_5 = 0.03125 gives experimental order of convergence p =
3.036056209583162
```

c) We will finally test both methods on the ODE

$$y'(t) = -2ty(t), \qquad y(0) = 1, \quad t \in [0, 0.5].$$

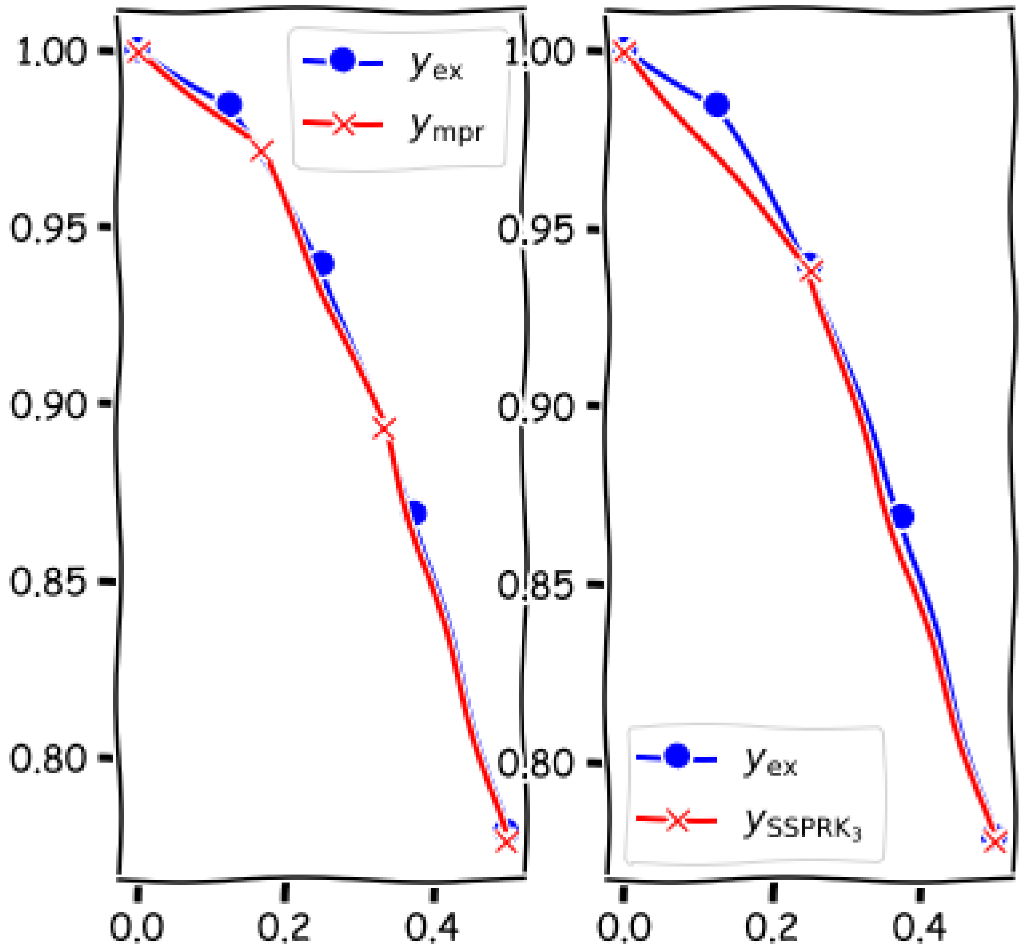
This has exact solution e^{-t^2}. Find the approximate value of $y(0.5)$ using * The midpoint method with $N_{max} = 3$ * The SSPRK3 method with $N_{max} = 2$

The number of step sizes are chosen such that each method needs to perform 6 evaluations of the function f. How do the errors $e = |y(T) - y_{N_{max}}|$ compare?

Additional exercise: Does this observation holds for other values of T? For instance, with $T = 0.2$ or $T = 0.8$. Can you tell what happens to y or y' in $T = 0.5$?

[78]:
```python
# defining the exact solution
def y_ex(t):
    return np.exp(-t**2)

# defining g (right hand side of the equation)
def g(t, y):
    return -2*t*y

# initial values
y0 = 1
t0 = 0
T = 0.5
N_max_mpr = 3
N_max_ssprk = 2

# solving the IVP
ts_mpr, ys_mpr = explicit_midpoint_rule(y0, t0, T, g, N_max_mpr)
ts_ssprk, ys_ssprk = explicit_ssprk3(y0, t0, T, g, N_max_ssprk)

x = np.linspace(0, 0.5, 5)
ys_ex = []
for val in x:
    ys_ex.append(y_ex(val))


fig, axes = plt.subplots(1,2)
axes[0].plot(x, ys_ex, 'bo-')
axes[0].plot(ts_mpr, ys_mpr, 'rx-')
axes[0].legend(["$y_{\mathrm{ex}}$", "$y_{\mathrm{mpr}}$" ])
ts, ys_ssprk3 = explicit_ssprk3(y0, t0, T, f, N_max)
axes[1].plot(x, ys_ex, 'bo-')
axes[1].plot(ts_ssprk, ys_ssprk, 'rx-')
axes[1].legend(["$y_{\mathrm{ex}}$", "$y_{\mathrm{SSPRK_3}}$" ])

e_mpr = np.absolute(y_ex(T) - ys_mpr[-1])
e_ssprk = np.absolute(y_ex(T) - ys_ssprk[-1])

print(f"Error for midpoint rule: e = {e_mpr}")
print(f"Error for SSPRK3: e = {e_ssprk}")
```

```
Error for midpoint rule: e = 0.002543491722271085
Error for SSPRK3: e = 0.0010497081744864634
```



1.0.3 Exercise 3

SIR Model The SIR model is a system of first order ODE's which model the dynamics of a disease in a society.

There are $S(t)$ susceptible/healthy individuals, $I(t)$ infected individuals and $R(t)$ recovered individuals. Each susceptible person has a risk of becoming infected, a risk which is proportional to the number of infected people $I(t)$, with a proportinality constant $\beta > 0$. Each infected person also has a chance of recovering, with a recovery constant $\gamma > 0$. This leads to the coupled system of first-order ODE's

$$\begin{aligned} S'(t) =& -\beta S(t)I(t), \\ I'(t) =& \beta S(t)I(t) - \gamma I(t), \\ R'(t) =& \gamma I(t). \end{aligned}$$

We can rewrite this in vector form as

$$\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t))$$

where we have defined

$$\mathbf{u}(t) = \begin{pmatrix} S(t) \\ I(t) \\ R(t) \end{pmatrix}, \quad \mathbf{f}(\mathbf{u}(t)) = \begin{pmatrix} -\beta S(t)I(t) \\ \beta S(t)I(t) - \gamma I(t) \\ \gamma I(t) \end{pmatrix}.$$

a) Show that the system is conservative, that is that the total number of individuals $S(t) + I(t) + R(t)$ is constant.

Hint: remember which is the derivative of a constant function.

If we add the 3 equations we will get:

$$S'(t) + I'(t) + R'(t) = -\beta S(t)I(t) + \beta S(t)I(t) - \gamma I(t) + \gamma I(t)$$

$$S'(t) + I'(t) + R'(t) = 0$$

If we now integrate on both sides we will get:

$$S(t) + I(t) + R(t) = \int_0^\infty 0 dt$$

$$S(t) + I(t) + R(t) = C$$

, where C is a constant, S is the antiderivative of $S'(t)$, I is the antiderivative of $I'(t)$ and R is the antiderivative of $R'(t)$. This shows that the sum of these 3 functions will always be a constant.

b) Numerically solve the system

$$\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t)), \quad \mathbf{u}(0) = \mathbf{u}_0, \quad t \in [0, T]$$

with either of the RK-methods above.

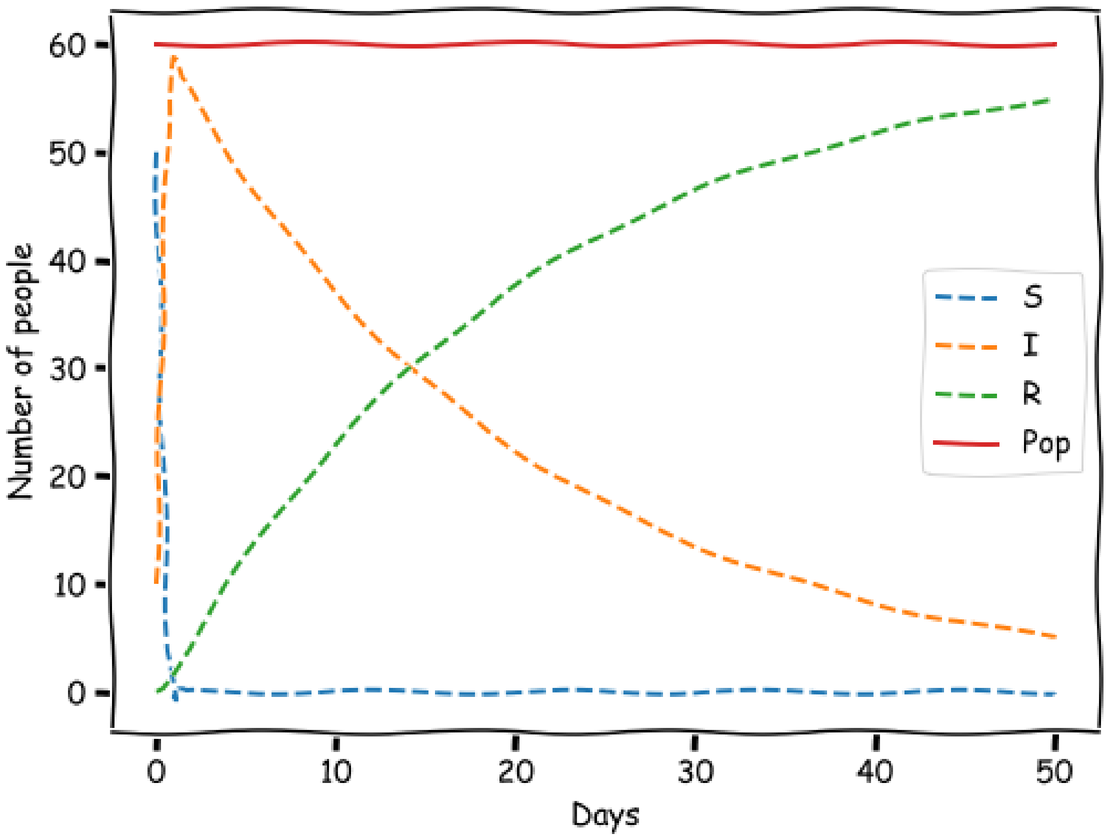
- You may pick end-time T and N_{max},
- Choose an initial number of individuals.
  - A suitable inital conditions could e.g. be $\mathbf{u}_0 = (50, 10, 0)^T$.
- Plot the solution as a function of time.
- Also plot the total number of individuals.
  - Is the total number conserved? To check this, you might calculate the maximum total and the minimum total over the interval.
- The parameters $\beta = 0.2$ and $\gamma = 0.15$ can be helpful for ilustration.

If you need a guide for this problem, you can look at the Lotka-Volterra model. It was presented in the lectures and is also available in the learning material on the wiki-page.

[79]:
```
T = 50
t0 = 0
I0 = 1/200000
S0 = 1 - I0
```

```python
R0 = 0
u0 = np.array([50, 10, 0])
N_max = 150
beta = 0.1
gamma = 0.05

def f(t, u):
    return np.array([-beta*u[0]*u[1],
                     beta*u[0]*u[1] - gamma*u[1],
                     gamma * u[1]
                    ])

def totalPopulation(u):
    return u[0] + u[1] + u[2]

ts, ys = explicit_ssprk3(u0, t0, T, f, N_max)
pop = np.zeros(len(ys))
ts_pop = np.zeros(len(ys))
for i in range(len(ys)):
    ts_pop[i] = ts[i]
    pop[i] = totalPopulation(ys[i])

newparams['figure.figsize'] = (8,6)
plt.rcParams.update(newparams)
plt.plot(ts, ys, "--")
plt.plot(ts_pop, pop, "-")
plt.legend(["S", "I", "R", "Pop"])
plt.xlabel("Days")
plt.ylabel("Number of people")
```

[79]: Text(0, 0.5, 'Number of people')



Additional exercise: modify the SIR model such that the population is not longer constant. One idea is to have a proportion of the infected population to die with rate δ. Test the new model as before.

```
[ ]:
```