A2

May 9, 2024

1 Computational Physics Blatt 04

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[ ]:
```
import numpy as np
from numpy.linalg import norm
from functools import partial
import matplotlib.pyplot as plt
import matplotlib
from scipy.optimize import curve_fit
from scipy.stats import linregress

matplotlib.rcParams["figure.figsize"] = [12, 8]
%matplotlib inline

T_MAX = 100 # Increased for nicer results
H = 0.001 # decreased for nicer results
SIGMA = 10
B = 8/3
R = 28
```

1.1 a)

Implementation of Runge-Kutta 5

[ ]:
```
def RKDP(f, y0, t0, tmax, h, digits=None, **kwargs):
    dim = len(y0)
    coef = {  # Coefficients for the Dormand-Prince method, padded with zeros␣
↪for the 6th order
        "k2": np.array([1 / 5, 0, 0, 0, 0, 0]).reshape(-1, 1),
        "k3": np.array([3 / 40, 9 / 40, 0, 0, 0, 0]).reshape(-1, 1),
        "k4": np.array([44 / 45, -56 / 15, 32 / 9, 0, 0, 0]).reshape(-1, 1),
        "k5": np.array(
            [19372 / 6561, -25360 / 2187, 64448 / 6561, -212 / 729, 0, 0]
        ).reshape(-1, 1),
        "k6": np.array(
            [9017 / 3168, -355 / 33, 46732 / 5247, 49 / 176, -5103 / 18656, 0]
        ).reshape(
```

```
            -1, 1
        ),  # called a6 in the literature
        "y": np.array(
            [35 / 384, 0, 500 / 1113, 125 / 192, -2187 / 6784, 11 / 84]
        ).reshape(
            -1, 1
        ),  # called b in the literature
        "t": np.array(
            [0, 1 / 5, 3 / 10, 4 / 5, 8 / 9, 1]
        ),  # called c in the literature
    }

    t = t0
    y = y0
    fp = partial(f, **kwargs)  # set sigma, r and b
    while t < tmax:
        ks = np.zeros((6, dim))
        ks[0] = h * fp(t, y)
        ks[1] = h * fp(t + h * coef["t"][1], y + np.sum(ks * coef["k2"]))
        ks[2] = h * fp(t + h * coef["t"][2], y + np.sum(ks * coef["k3"]))
        ks[3] = h * fp(t + h * coef["t"][3], y + np.sum(ks * coef["k4"]))
        ks[4] = h * fp(t + h * coef["t"][4], y + np.sum(ks * coef["k5"]))
        ks[5] = h * fp(t + h * coef["t"][5], y + np.sum(ks * coef["k6"]))
        y += np.sum(coef["y"] * ks, axis=0)
        if digits:
            y = np.round(y, digits)
        t += h
        yield t, *y
```

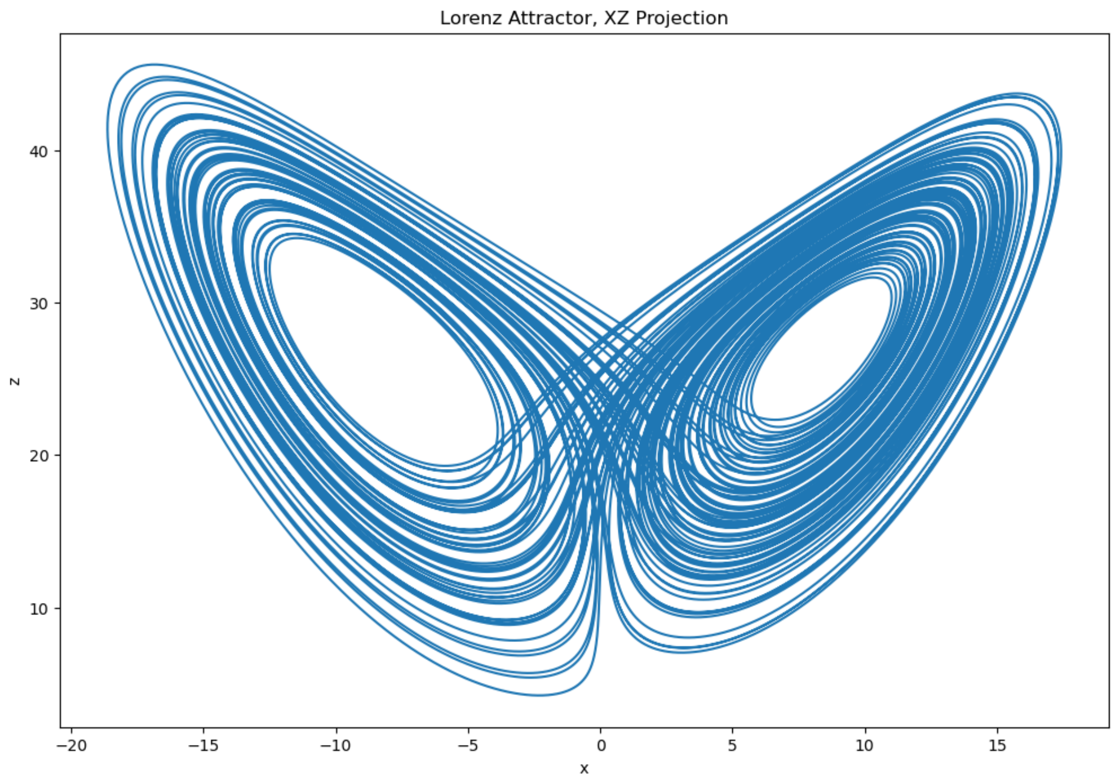
1.2 b)

Solve the Lorenz equation with $y_0 = (2, 3, 14)$, the parameters $\sigma = 10$, $b = \frac{3}{5}$ and $r = 28$ in the time frame $t_0 = 0$ to $t_e = 50$ with a stepsize of $h = 0.01$. Plot the XZ-projection.

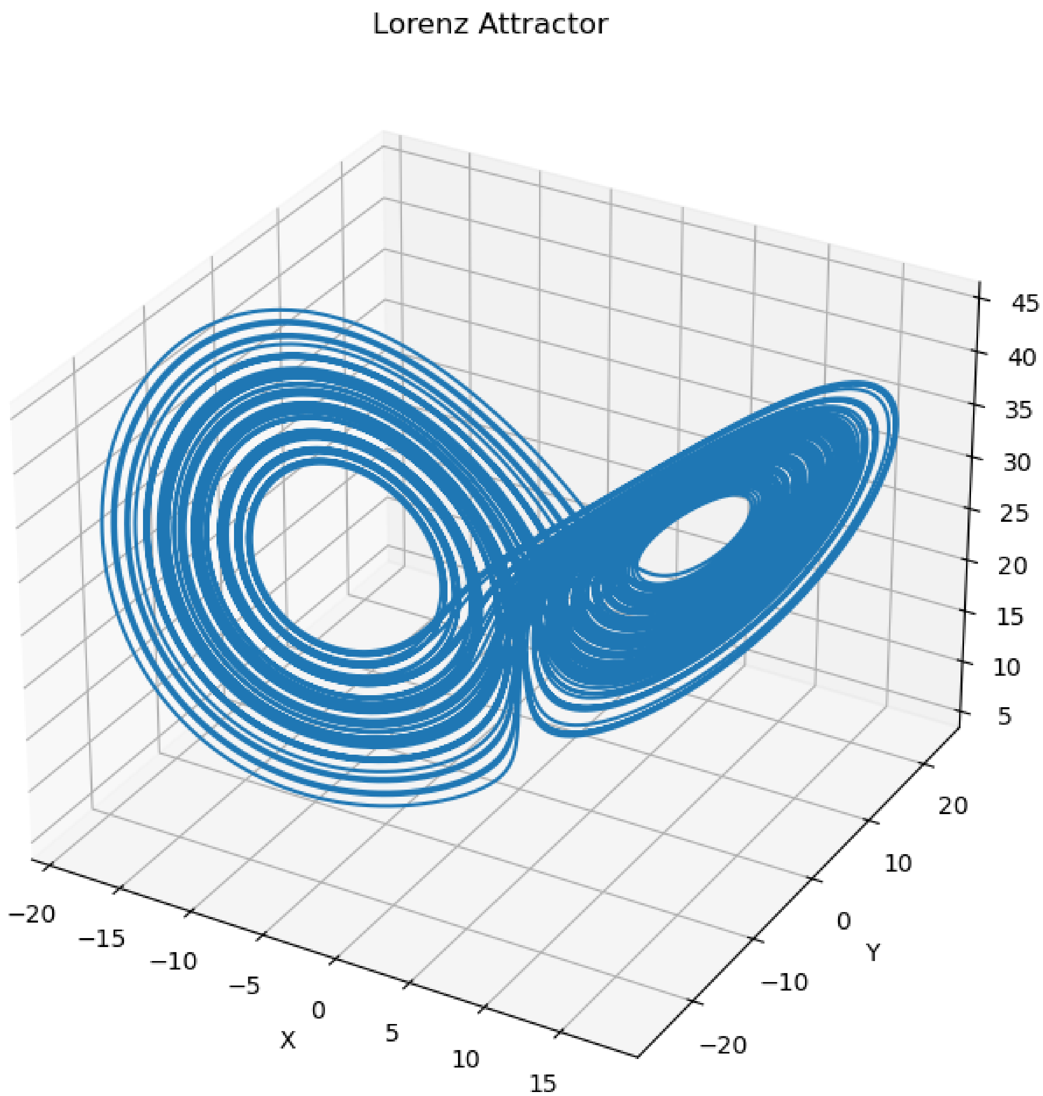
[ ]:
```
def lorentz(t, y, sigma, r, b):
    x_dot = sigma * (y[1] - y[0])
    y_dot = y[0] * (r - y[2]) - y[1]
    z_dot = y[0] * y[1] - b * y[2]
    return np.array([x_dot, y_dot, z_dot])
```

[ ]:
```
y0 = np.array([2, 3, 14], dtype=float)  # prevent type-casting errors
rkdp = RKDP(lorentz, y0, t0=0, tmax=T_MAX, h=H, sigma=SIGMA, r=R, b=B)
system = np.array(list(rkdp))
time = system[:, 0]
trajectory = system[:, 1:]
```

[ ]:
```python
plt.plot(trajectory[:, 0], trajectory[:, 2])
plt.xlabel("x")
plt.ylabel("z")
plt.title("Lorenz Attractor, XZ Projection")
None  # prevent ugly output
```



[ ]:
```python
fig = plt.figure()
ax = fig.add_subplot(1, 1, 1, projection="3d")

ax.plot(trajectory[:, 0], trajectory[:, 1], trajectory[:, 2])
ax.set_xlabel("X")
ax.set_ylabel("Y")
ax.set_zlabel("Z")  # strangly missing
plt.title("Lorenz Attractor")
None  # prevent ugly output
```



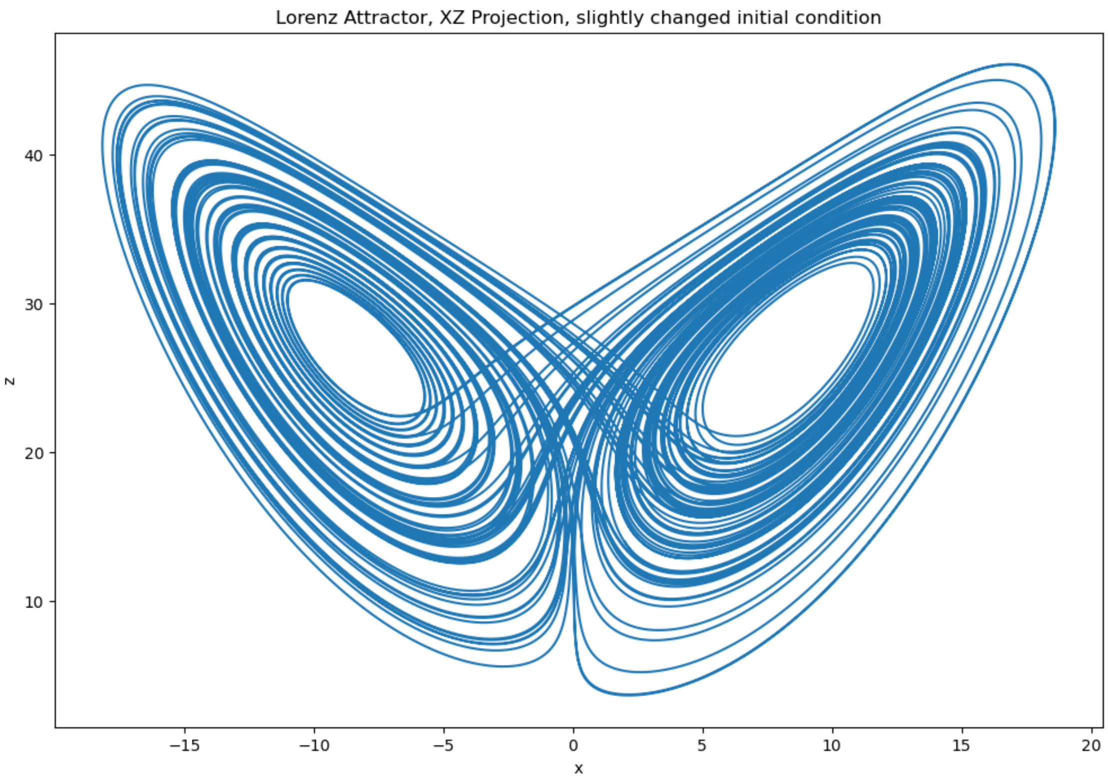
1.3 c)

Check the chaotic nature by using $y_0 = (2, 3, 14 + 10^{-9})$ and compare the trajectories.

[ ]:
```
y0_eps = np.array([2, 3, 14 + 1e-9], dtype=np.float64)
rkdp2 = RKDP(lorentz, y0_eps, t0=0, tmax=T_MAX, h=H, sigma=SIGMA, r=R, b=B)
system2 = np.array(list(rkdp2))
time2 = system2[:, 0]
trajectory2 = system2[:, 1:]
```

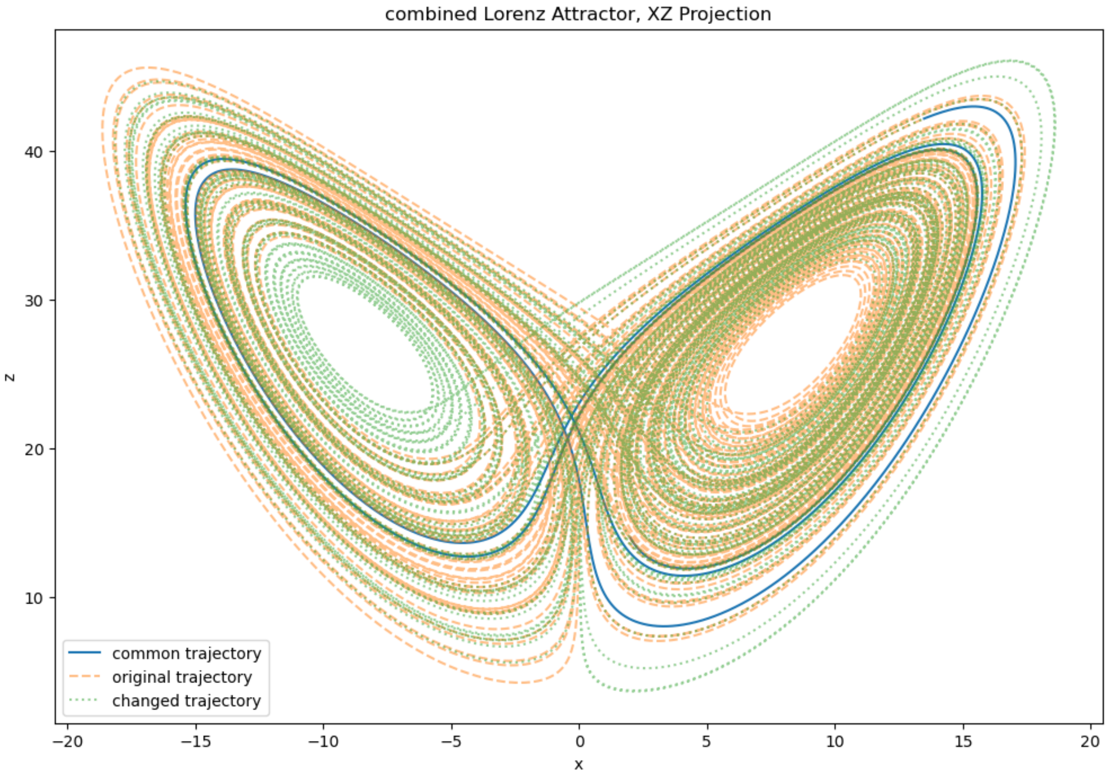
[ ]:
```
plt.plot(trajectory2[:, 0], trajectory2[:, 2])
plt.xlabel("x")
```

```python
plt.ylabel("z")
plt.title("Lorenz Attractor, XZ Projection, slightly changed initial condition")
None  # prevent ugly output
```



[ ]:
```python
traj_mask = np.all(np.isclose(trajectory, trajectory2, rtol=1e-7), axis=1)
div_point = np.argmin(traj_mask)
plt.plot(
    trajectory[:div_point, 0],
    trajectory[:div_point, 2],
    ls="solid",
    label="common trajectory",
)
plt.plot(
    trajectory[div_point:, 0],
    trajectory[div_point:, 2],
    ls="dashed",
    alpha=0.5,
    label="original trajectory",
)
plt.plot(
    trajectory2[div_point:, 0],
    trajectory2[div_point:, 2],
```

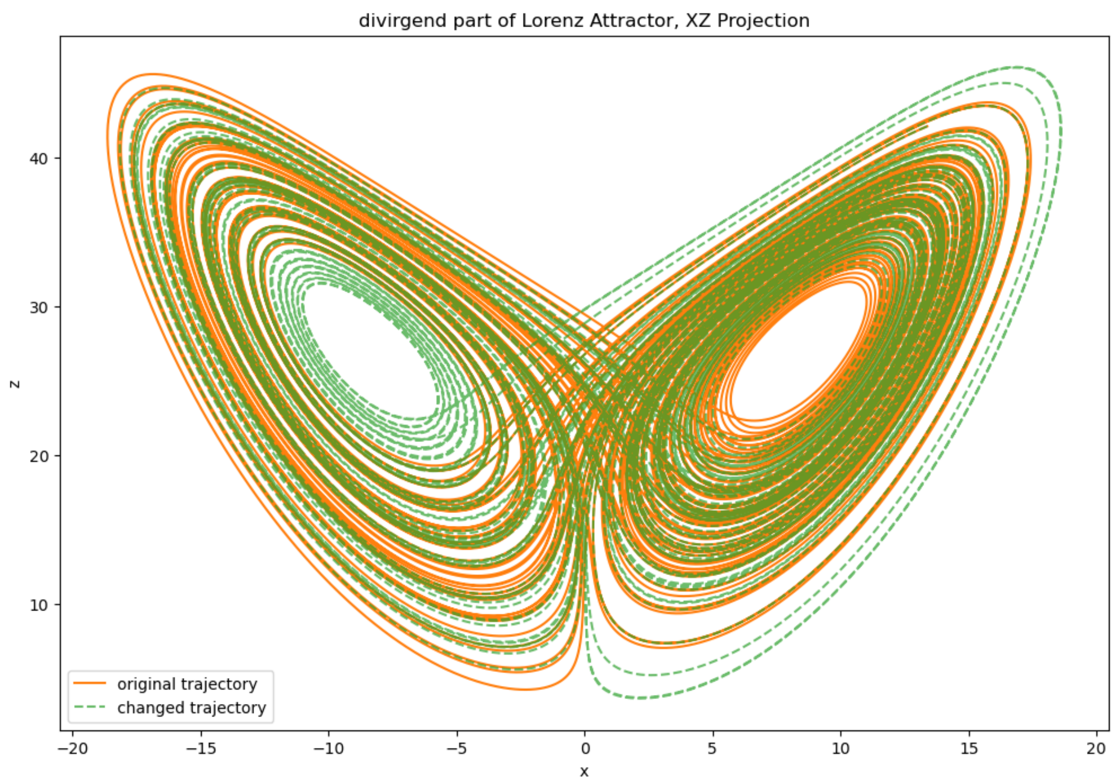
```
    ls="dotted",
    alpha=0.5,
    label="changed trajectory",
)
plt.legend()
plt.xlabel("x")
plt.ylabel("z")
plt.title("combined Lorenz Attractor, XZ Projection")
None  # prevent ugly output
```



[ ]:

```
plt.plot(
    trajectory[div_point:, 0],
    trajectory[div_point:, 2],
    ls="solid",
    c="tab:orange",
    label="original trajectory",
)
plt.plot(
    trajectory2[div_point:, 0],
    trajectory2[div_point:, 2],
    ls="dashed",
    c="tab:green",
```

```
    alpha=0.7,
    label="changed trajectory",
)
plt.legend()
plt.xlabel("x")
plt.ylabel("z")
plt.title("divirgend part of Lorenz Attractor, XZ Projection")
None  # prevent ugly output
```



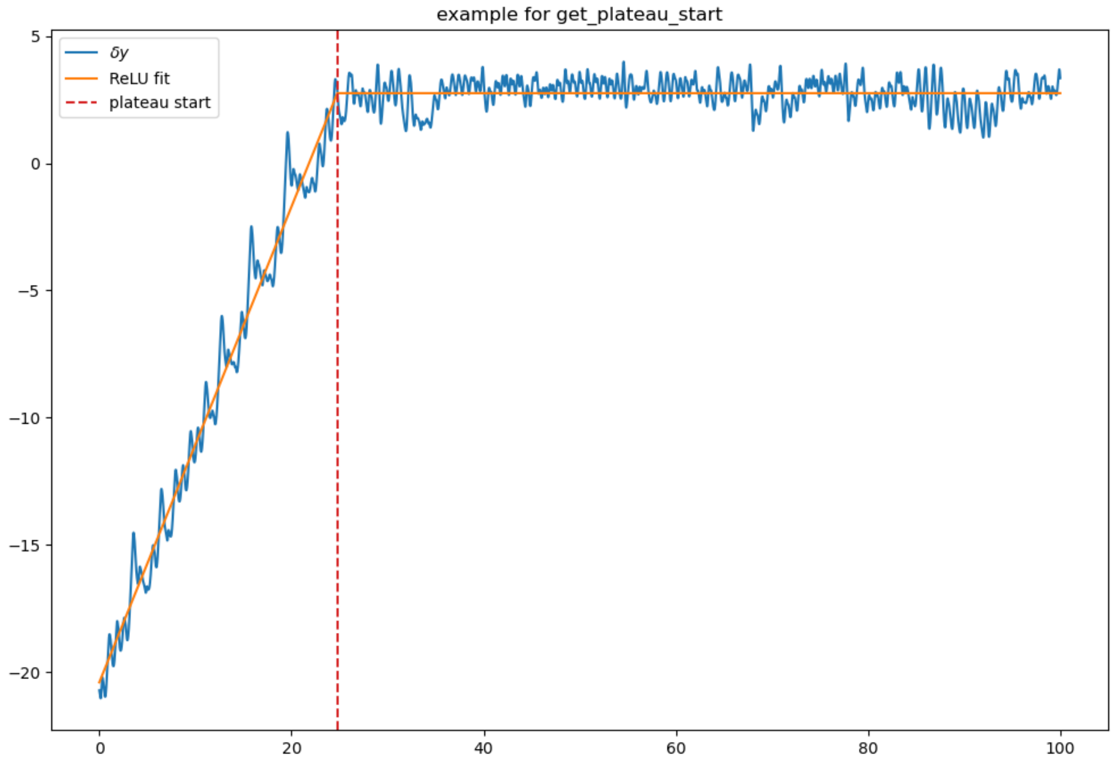
1.4 d)

Calculate the Liapunov exponent. Plot the result and create a fit to an exponential function.

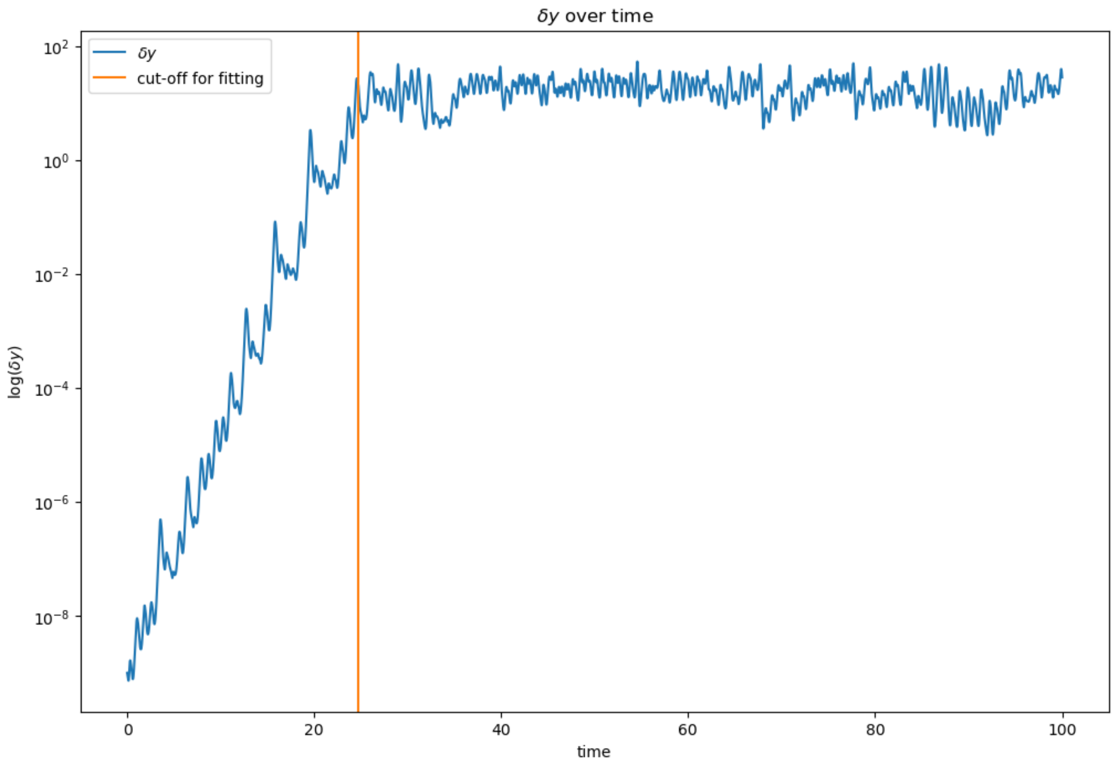
[ ]:
```
delta_y = np.linalg.norm(trajectory2 - trajectory, axis=1)


def liapunov(t, lambda_, a):
    return np.exp(lambda_ * t) * a
```

[ ]:
```
```

```python
# automation for the search of the plateau start by fitting a function to the␣
↪data. This only works if the data has the increas-plateau form. If not␣
↪return NaN. As the min and max value are already good estimations for b and␣
↪c, this fit should converge rather quickly.


def relu(x, a, b, c):
    return np.minimum(a * x + b, c)


def get_plateau_start(
    delta_y, time
):  # This was way more work than doing part f) by hand
    """Fitts a relu function to the data and returns the time at which the␣
↪function plateaus."""
    logY = np.log(delta_y)
    try:
        params, cov = curve_fit(
            relu,
            time[delta_y > 0],
            logY[delta_y > 0],
            p0=[1, np.min(logY), np.max(logY)],
        )
        t_cutoff = (params[2] - params[1]) / params[0]  # x = (c-b)/a
    except RuntimeError:  # if the fit fails, return nan
        t_cutoff = np.nan
    return t_cutoff


# example plot of what we are doing
logY = np.log(delta_y)
params, cov = curve_fit(relu, time, logY, p0=[1, np.min(logY), np.max(logY)])
plt.plot(time, np.log(delta_y), label="$\delta y$")
plt.plot(time, relu(time, *params), label="ReLU fit")
plt.axvline(
    get_plateau_start(delta_y, time), c="tab:red", ls="--", label="plateau␣
↪start"
)
plt.legend()
plt.title("example for get_plateau_start")
None  # prevent ugly output
```



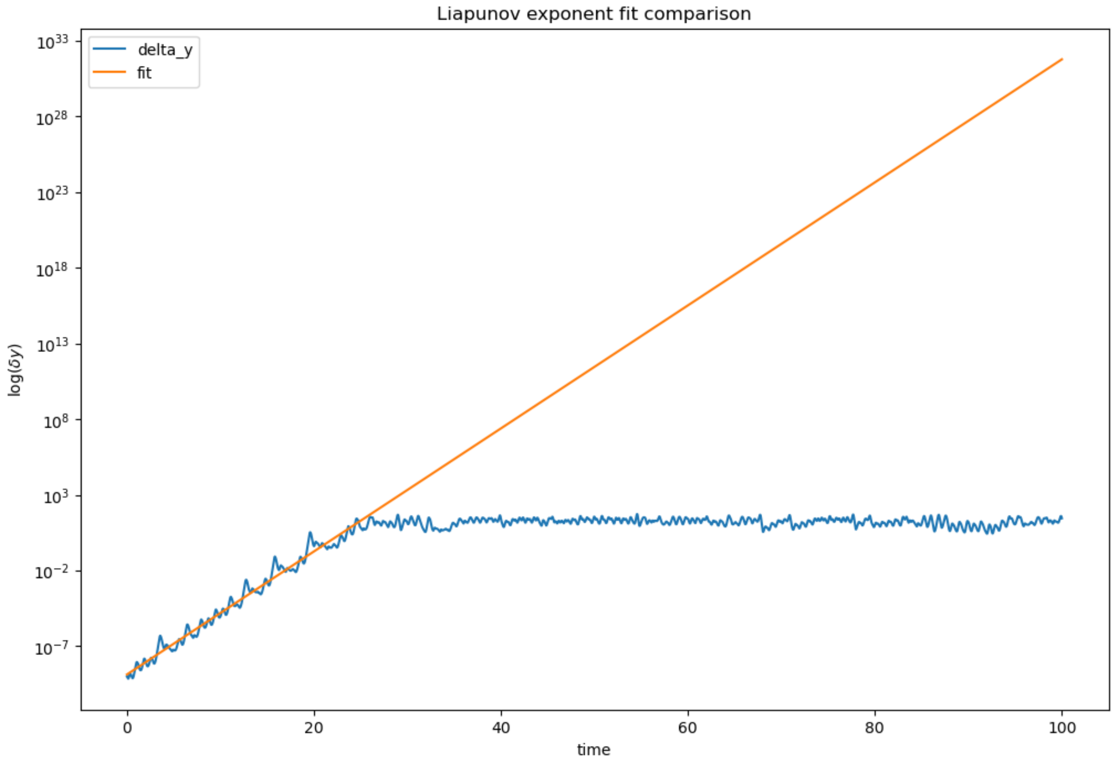
[ ]:
```
delta_y = np.linalg.norm(trajectory2 - trajectory, axis=1)
t_cutoff = get_plateau_start(delta_y, time)

plt.plot(time, delta_y, label="$\delta y$")
plt.yscale("log")
plt.ylabel(r"log($\delta y$)")
plt.axvline(x=t_cutoff, c="tab:orange", label="cut-off for fitting")
plt.xlabel("time")
plt.title("$\delta y$ over time")
plt.legend()
None  # prevent ugly output
```




```
[ ]: linFit = linregress(
         time[time < t_cutoff], np.log(delta_y[time < t_cutoff])
     )  # if a linear regression is possible, it performs better than an ordinary␣
      ↪minimizer
     print(f"Lyapunov exponent: {linFit.slope}")
     print(f"a value: {np.exp(linFit.intercept)}")
```

```
Lyapunov exponent: 0.9357312391505839
a value: 1.3669578951590576e-09
```

```
[ ]: plt.plot(time, delta_y, label="delta_y")
     plt.plot(time, liapunov(time, linFit.slope, np.exp(linFit.intercept)),␣
      ↪label="fit")
     plt.yscale("log")
     plt.ylabel(r"log($\delta y$)")
     plt.xlabel("time")
     plt.legend()
     plt.title("Liapunov exponent fit comparison")
     None  # prevent ugly output
```



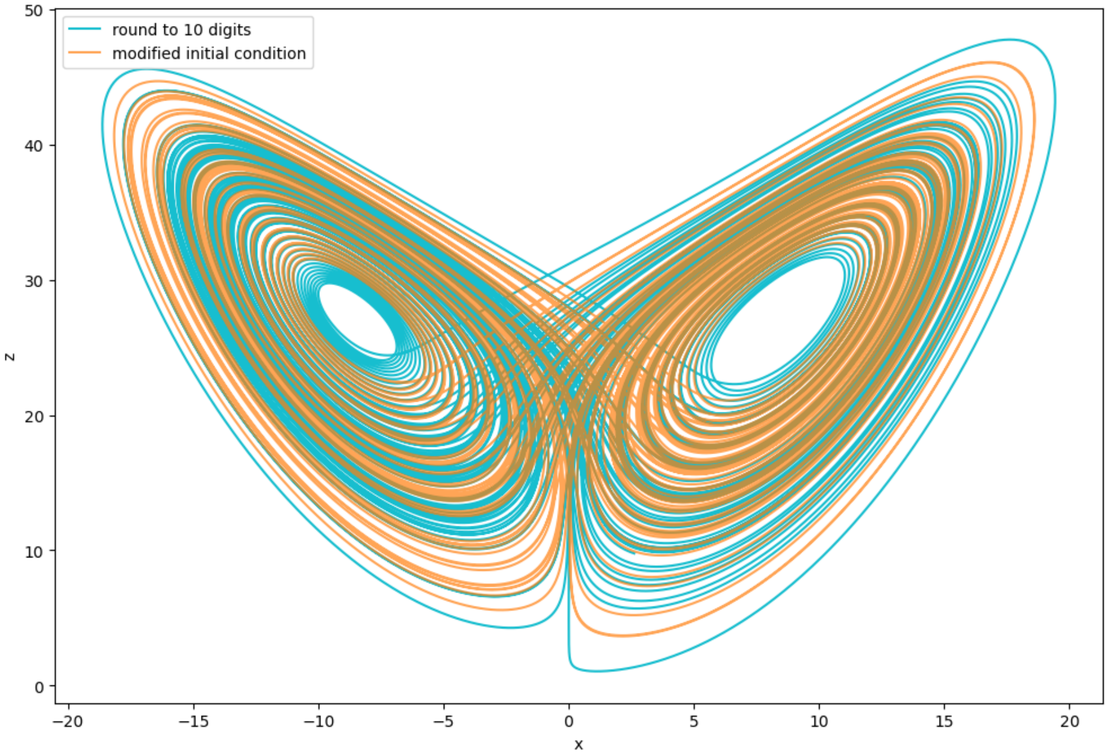
1.5 e)

Create errors by rounding the values to 10 digits. Compare them to the trajectory from b).

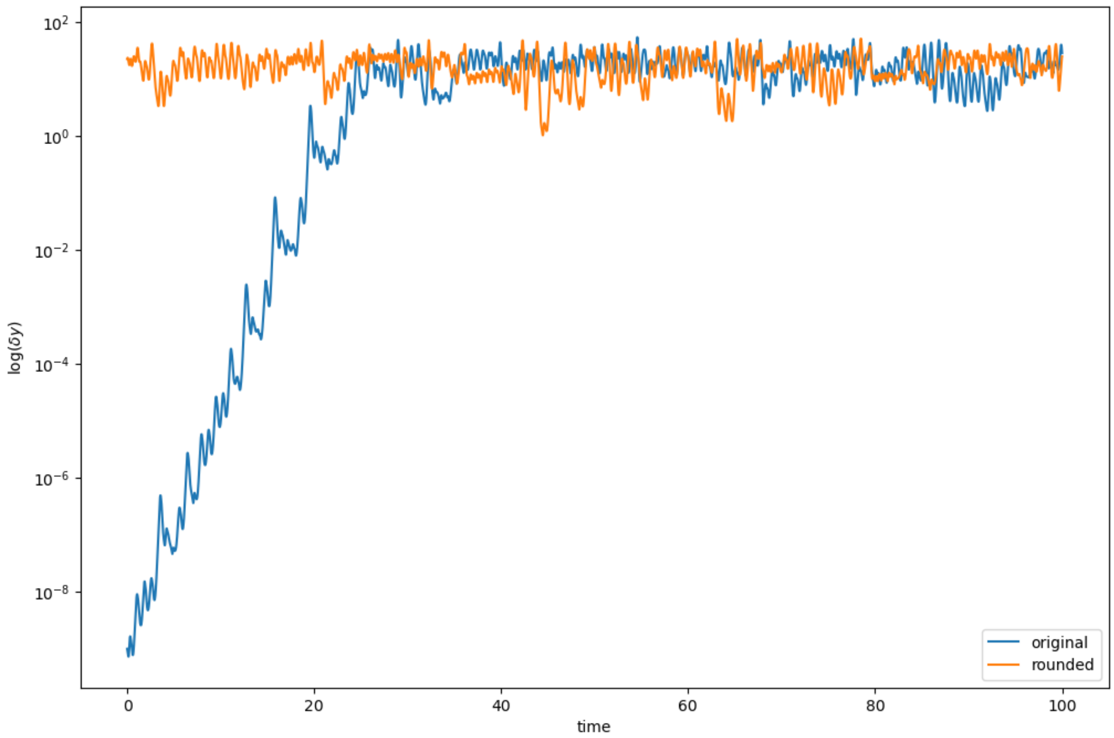
[ ]:
```
rkdp3 = RKDP(
    lorentz,
    y0,
    t0=0,
    tmax=T_MAX,
    h=H,
    digits=10,
    sigma=SIGMA,
    r=R,
    b=B,
)
system3 = np.array(list(rkdp3))
time3 = system3[:, 0]
trajectory3 = system3[:, 1:]
```

[ ]:
```
plt.plot(trajectory3[:, 0], trajectory3[:, 2], c="tab:cyan", label="round to 10␣
↪digits")
plt.plot(
    trajectory2[:, 0],
```

```
    trajectory2[:, 2],
    c="tab:orange",
    label="modified initial condition",
    alpha=0.7,
)
plt.legend()
plt.xlabel("x")
plt.ylabel("z")
None  # prevent ugly output
```



[ ]:
```
delta_y3 = np.linalg.norm(trajectory3 - trajectory, axis=1)

plt.plot(time, delta_y, label="original")
plt.plot(time, delta_y3, label="rounded")
plt.yscale("log")
plt.ylabel(r"log($\delta y$)")
plt.xlabel("time")
plt.legend()
None  # prevent ugly output
```



When introducing errors due to rounding, δy stays in the same (big) order of magnitude. The "natural" divergence has an exponential increasing error instead.

1.6 f)

Lower r to find a r_{crit} where the system is no longer chaotic.

[ ]:
```
def liapFromLorePara(r, sigma, b, t0, tmax, h, digits=None):
    """calculates the liapunov exponent of the lorenz system for given␣
    ↪parameters."""
    y0 = np.array([2, 3, 14], dtype=float)  # prevent type-casting errors
    rkdp0 = RKDP(lorentz, y0, t0, tmax, h, digits=digits, sigma=sigma, r=r, b=b)
    system0 = np.array(list(rkdp0))
    time0 = system0[:, 0]
    trajectory0 = system0[:, 1:]

    y1 = np.array([2, 3, 14 + 1e-9], dtype=float)  # prevent type-casting errors
    rkdp1 = RKDP(lorentz, y1, t0, tmax, h, digits=digits, sigma=sigma, r=r, b=b)
    system1 = np.array(list(rkdp1))
    time1 = system1[:, 0]
    trajectory1 = system1[:, 1:]

    delta_y = np.linalg.norm(trajectory0 - trajectory1, axis=1)
    t_cutoff = get_plateau_start(delta_y, time0)
```

```
    if np.isnan(t_cutoff):
        return np.NaN
    if len(time0[time0 < t_cutoff]) < 2 or len(time0[time0 < t_cutoff]) == len(
        time0
    ):  # check if plateau start is in the time frame
        return 0
    linFit = linregress(time0[time0 < t_cutoff], np.log(delta_y[time0 <␣
↪t_cutoff]))
    return linFit.slope
```

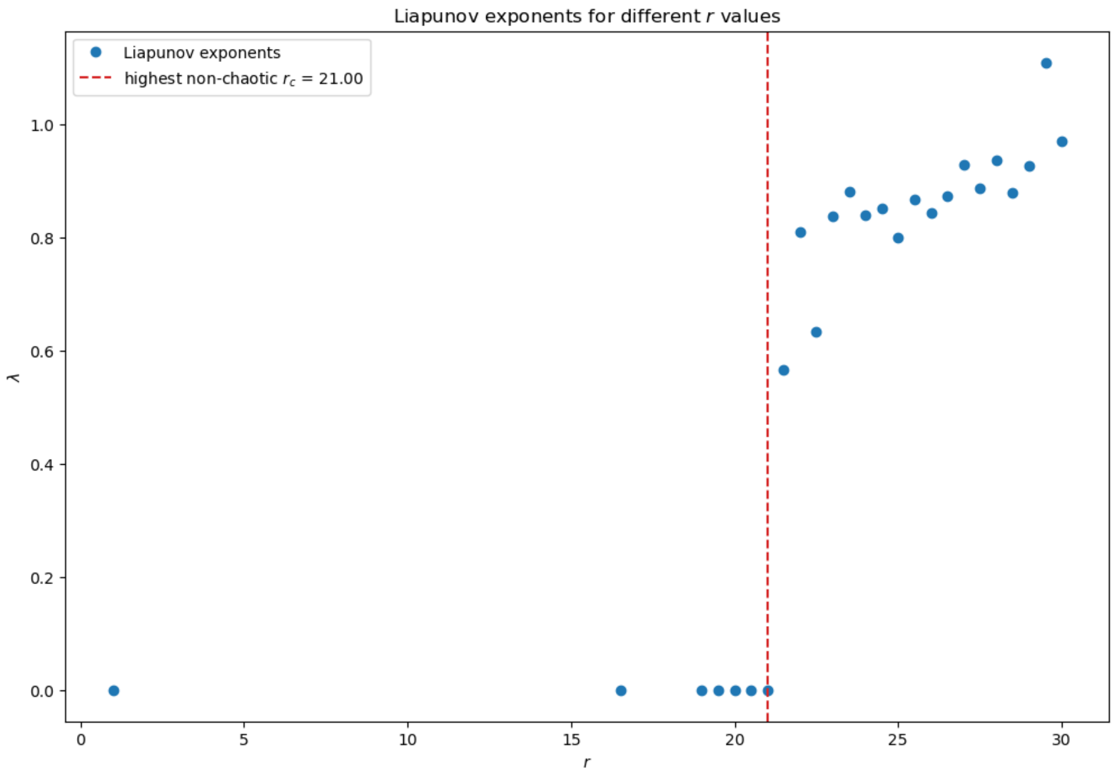
[ ]:
```
from multiprocessing import Pool, cpu_count


rs = np.linspace(1, 30, 59)

liapF = partial(liapFromLorePara, sigma=SIGMA, b=B, t0=0, tmax=T_MAX, h=H)


with Pool(cpu_count() - 2) as p:  # use all but 2 cores
    liap = np.array(p.map(liapF, rs))
```

```
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:14: OptimizeWarning: Covariance of the
parameters could not be estimated
  params, cov = curve_fit(
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
```

```
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:12: RuntimeWarning: divide by zero
encountered in log
  logY = np.log(delta_y)
/tmp/ipykernel_16137/1903625063.py:14: OptimizeWarning: Covariance of the
parameters could not be estimated
  params, cov = curve_fit(
/tmp/ipykernel_16137/1903625063.py:14: OptimizeWarning: Covariance of the
parameters could not be estimated
  params, cov = curve_fit(
/tmp/ipykernel_16137/1903625063.py:14: OptimizeWarning: Covariance of the
parameters could not be estimated
  params, cov = curve_fit(
```

[ ]:

```
r_crit = rs[liap == 0][-1]
plt.plot(rs, liap, marker="o", ls="none", label="Liapunov exponents")
plt.axvline(
    r_crit, c="tab:red", ls="--", label=f"highest non-chaotic $r_c$ = {r_crit:.
 ↪2f}"
)
plt.xlabel("$r$")
plt.ylabel("$\lambda$")
plt.legend()
plt.title("Liapunov exponents for different $r$ values")
None  # prevent ugly output
```



1.7 g)

Implement the dynamic step-size using a safety factor of $S = 0.95$. Compare the compute time to the fixed approach.

[ ]:

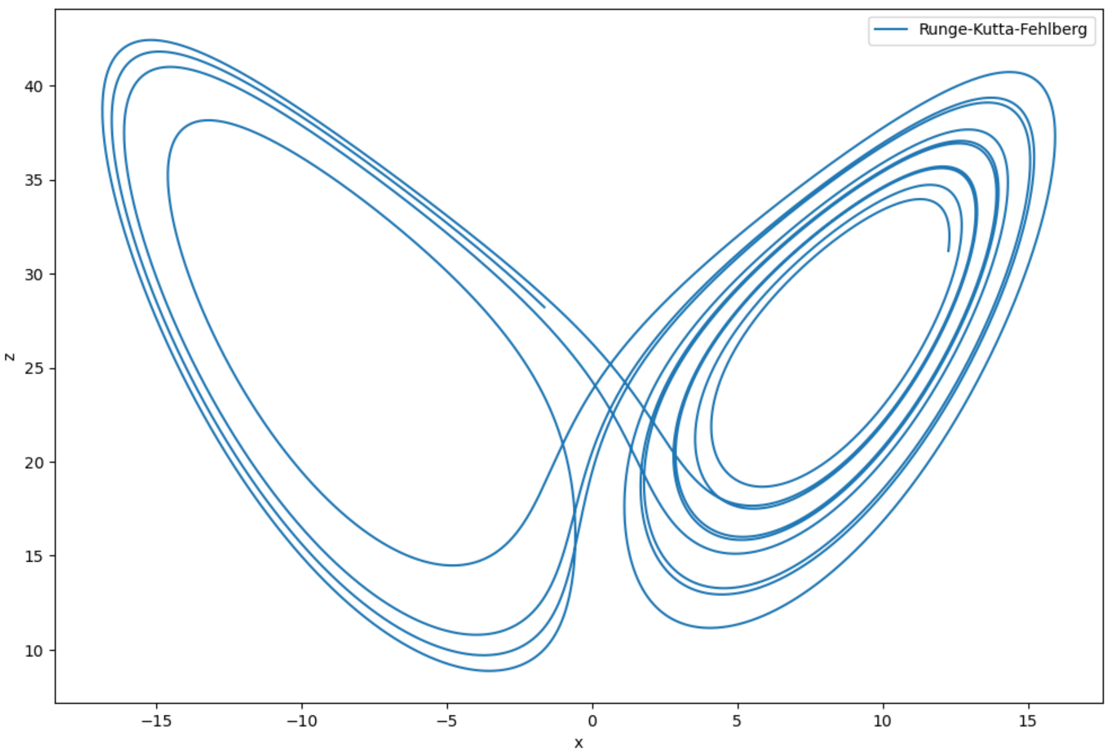
```
def RKF(f, y0, t0, tmax, h0, atol, rtol, hmax, S=0.95, alpha=0.2, **kwargs):
    dim = len(y0)
    coef = {  # Coefficients for the Dormand-Prince method, padded with zeros␣
↪for the 6th order
        "k2": np.array([1 / 5, 0, 0, 0, 0, 0]).reshape(-1, 1),
        "k3": np.array([3 / 40, 9 / 40, 0, 0, 0, 0]).reshape(-1, 1),
        "k4": np.array([44 / 45, -56 / 15, 32 / 9, 0, 0, 0]).reshape(-1, 1),
        "k5": np.array(
            [19372 / 6561, -25360 / 2187, 64448 / 6561, -212 / 729, 0, 0]
        ).reshape(-1, 1),
        "k6": np.array(
            [9017 / 3168, -355 / 33, 46732 / 5247, 49 / 176, -5103 / 18656, 0]
        ).reshape(
            -1, 1
        ),  # called a6 in the literature
        "y5": np.array(
            [35 / 384, 0, 500 / 1113, 125 / 192, -2187 / 6784, 11 / 84]
```

```
        ).reshape(
            -1, 1
        ),  # called b in the literature
        "y4": np.array(
            [5179 / 57600, 0, 7571 / 16695, 393 / 640, -92097 / 339200, 187 / 2100]
        ).reshape(
            -1, 1
        ),  # called b* in the literature
        "t": np.array(
            [0, 1 / 5, 3 / 10, 4 / 5, 8 / 9, 1]
        ),  # called c in the literature
    }

    t = t0
    y = y0
    h = h0
    fp = partial(f, **kwargs)
    while t < tmax:
        ks = np.zeros((6, dim))
        ks[0] = h * fp(t, y)
        ks[1] = h * fp(t + h * coef["t"][1], y + np.sum(ks * coef["k2"]))
        ks[2] = h * fp(t + h * coef["t"][2], y + np.sum(ks * coef["k3"]))
        ks[3] = h * fp(t + h * coef["t"][3], y + np.sum(ks * coef["k4"]))
        ks[4] = h * fp(t + h * coef["t"][4], y + np.sum(ks * coef["k5"]))
        ks[5] = h * fp(t + h * coef["t"][5], y + np.sum(ks * coef["k6"]))
        y5 = np.sum(coef["y5"] * ks, axis=0)
        y4 = np.sum(coef["y4"] * ks, axis=0) + y5 / 40
        scale = atol + rtol * np.max([norm(y), norm(y5)], axis=0)
        err = np.sqrt(np.mean(((y5 - y4) / scale) ** 2))

        if err < 1:
            t += h
            h = np.min(
                [S * h * (1 / err) ** alpha, hmax]
            )  # here we check for the maximum step size
            y += y5
            yield t, *y
        else:
            h = S * h * (1 / err) ** alpha
```

[ ]:
```
rkf = RKF(
    lorentz,
    y0,
    t0=0,
    tmax=10,
    h0=0.01,
```

```
    hmax=2,
    atol=1e-8,  # 1e-12 takes way too long
    rtol=1e-8,  # took around 10 minutes
    sigma=SIGMA,
    r=R,
    b=B,
)
system_rkf = np.array(list(rkf))
time_rkf = system_rkf[:, 0]
trajectory_rkf = system_rkf[:, 1:]
```

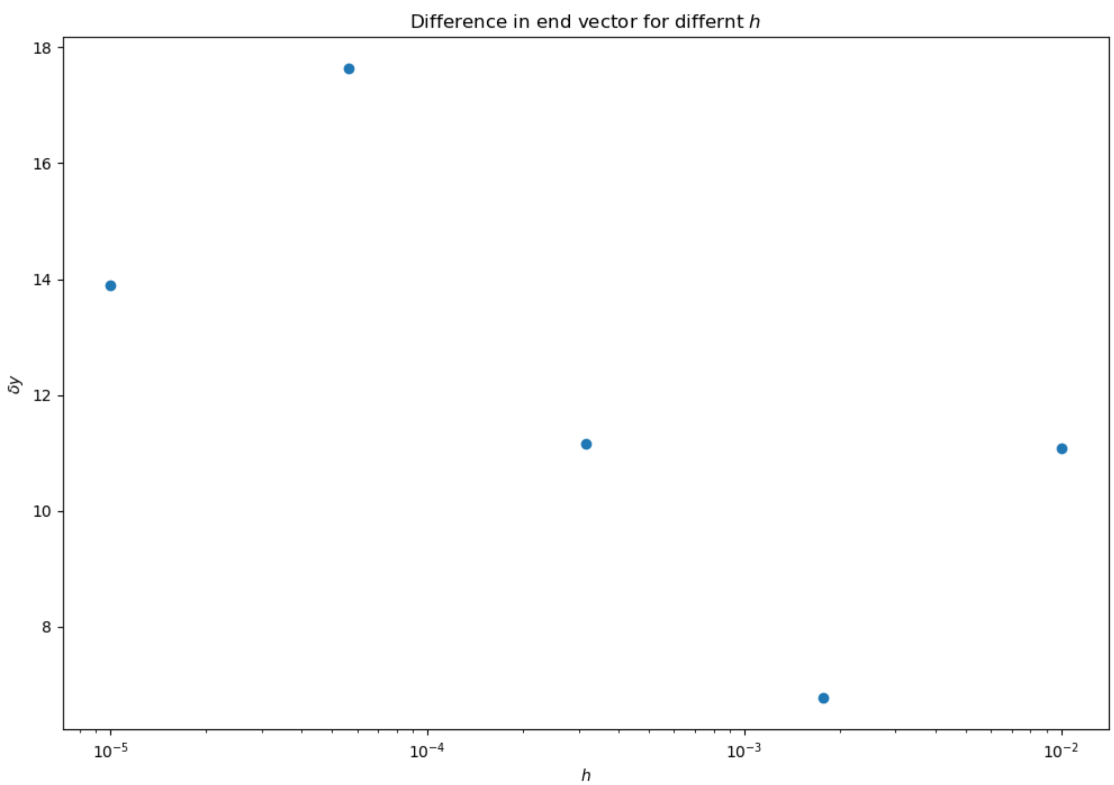
[ ]:
```
plt.plot(trajectory_rkf[:, 0], trajectory_rkf[:, 2],␣
 ↪label="Runge-Kutta-Fehlberg")
plt.legend()
plt.xlabel("x")
plt.ylabel("z")
None  # prevent ugly output
```



[ ]:
```
hs = np.logspace(-5, -2, 5)


def hToDeltaY(h):
```

```
    rkdp_ = RKDP(lorentz, y0, t0=0, tmax=10, h=h, sigma=SIGMA, r=R, b=B)
    system_ = np.array(list(rkdp_))
    time_temp = system_[:, 0]
    trajectory_ = system_[:, 1:]
    return (norm(trajectory_[-1] - trajectory_rkf[-1]), h)


with Pool(cpu_count() - 2) as p:  # use all but 2 cores
    pool_result = np.array(p.map(hToDeltaY, hs))
```

[ ]:
```
plt.scatter(pool_result[:, 1], pool_result[:, 0])
plt.xscale("log")
plt.xlabel("$h$")
plt.ylabel("$\delta y$")
plt.title("Difference in end vector for differnt $h$")
None  # prevent ugly output
```



We are not even close to $\delta y(t_e) < 10^{-6}$. But reducing h any more leeds to unreasonable computation time. We might have an error in this implementation.