

Question 1

a)

We can approximate a derivative with two points using a derivative to the left, and one to the right using

$$f'(x) = \frac{f(x + \delta) - f(x - \delta)}{2\delta},$$

or

$$f'(x) = \frac{f(x + 2\delta) - f(x - 2\delta)}{4\delta},$$

In this problem, I will use the four points $x \pm \delta$ and $x \pm 2\delta$ to approximate the derivative,

To approximate this, we can Taylor expand it:

$$f(x \pm \delta) = f(x) \pm \delta f'(x) + \frac{1}{2}\delta^2 f''(x) \pm \frac{1}{3!}\delta^3 f'''(x) + \frac{1}{4!}\delta^4 f^{(4)}(x) \pm \frac{1}{5!}\delta^5 f^{(5)}(x) + \dots$$

Similarly, for $f(x \pm 2\delta)$:

$$f(x \pm 2\delta) = f(x) \pm 2\delta f'(x) + \frac{2^2}{2}\delta^2 f''(x) \pm \frac{2^3}{3!}\delta^3 f'''(x) + \frac{2^4}{4!}\delta^4 f^{(4)}(x) \pm \frac{2^5}{5!}\delta^5 f^{(5)}(x) + \dots$$

This is awful, but we can cancel out some terms: all the non \pm terms will go away if we do $f(x + \delta) - f(x - \delta)$ and $f(x + 2\delta) - f(x - 2\delta)$ so let's do it. We have:

$$f(x + \delta) - f(x - \delta) \approx 2\delta f'(x) + \frac{1}{3}\delta^3 f'''(x) + \frac{1}{60}\delta^5 f^{(5)}(x), \quad (1)$$

and

$$f(x + 2\delta) - f(x - 2\delta) = 4\delta f'(x) + \frac{8}{3}\delta^3 f'''(x) + \frac{8}{15}\delta^5 f^{(5)}(x), \quad (2)$$

where I have truncated after the 5th order. We can get a better estimate of $f'(x)$ if we manage to cancel out the $f'''(x)$ term. We need a linear combination of the two derivatives such that:

$$a \left(\frac{f(x + \delta) - f(x - \delta)}{2\delta} \right) + b \left(\frac{f(x + 2\delta) - f(x - 2\delta)}{4\delta} \right) = \delta f'(x) + c\delta^5 f^{(5)}(x) \quad (3)$$

Putting Equations (1) and (2) in Equation (3) in this gives:

$$\begin{aligned} a \left(f'(x) + \frac{1}{6}\delta^2 f'''(x) + \frac{1}{120}\delta^4 f^{(5)}(x) \right) + b \left(\delta f'(x) + \frac{2}{3}\delta^3 f'''(x) + \frac{2}{15}\delta^5 f^{(5)}(x) \right) \\ = \delta f'(x) + c\delta^5 f^{(5)}(x). \end{aligned}$$

This gives the system of equations:

$$\frac{a}{6} + \frac{2b}{3} = 0$$

$$a + b = 1$$

Which has solutions $a = 4/3$ and $b = -1/3$, and this sets c to be $-1/30$. Plugging these values in Equation (3) yields:

$$\frac{4}{3} \left(\frac{f(x + \delta) - f(x - \delta)}{2\delta} \right) - \frac{1}{3} \left(\frac{f(x + 2\delta) - f(x - 2\delta)}{4\delta} \right) = f'(x) - \frac{1}{30} \delta^4 f^{(5)}(x),$$

and we can solve for $f'(x)$:

$$f'(x) = \frac{8(f(x + \delta) - f(x - \delta)) - (f(x + 2\delta) - f(x - 2\delta))}{12\delta} + \frac{1}{30} \delta^4 f^{(5)}(x). \quad (4)$$

The first term of Equation (4) is our estimate of the derivative, while the second term ($\Delta = \frac{1}{30} \delta^4 f^{(5)}(x)$) is the error.

b)

Now, to find the best δ possible we need to take into consideration the machine error, which I've ignored until now. In general, when considering the machine precision (ϵ), we get terms like $g_1 \epsilon f(x)/2\delta$ for Equation (1) and $g_2 \epsilon f(x)/4\delta$ for Equation (2). If we combine these terms together in the same linear combination as in (a) and add them to the error Δ , we get

$$\Delta = \frac{1}{30} \delta^4 f^{(5)}(x) + \frac{\epsilon g}{\delta} f(x), \quad (5)$$

where I've combined the g_1 , g_2 , and all the other constants into g . This is our error on the derivative, and what we want to minimize with respect to δ . So let's take the derivative and set it to zero:

$$\frac{d\Delta}{d\delta} = \frac{4}{30} \delta^3 f^{(5)}(x) - \frac{\epsilon g}{\delta^2} f(x) = 0,$$

$$\frac{4}{30} \delta^3 f^{(5)}(x) = \frac{\epsilon g}{\delta^2} f(x)$$

$$\delta^5 = \frac{15\epsilon g}{2} \frac{f(x)}{f^{(5)}(x)}$$

$$\delta \approx \left(\frac{15\epsilon}{2} \frac{f(x)}{f^{(5)}(x)} \right)^{1/5} \quad (6)$$

Since we work with exponentials in this question, we can set $f(x)/f^{(5)}(x) \approx 1$ since the derivatives of the exponentials look a lot like the exponentials. This gives us

$$\delta \approx \left(\frac{15\epsilon}{2} \right)^{1/5}, \quad (7)$$

and for double digit precision, $\epsilon = 1e16$. Demonstrations of this below and in q1.ipynb.

```
In [ ]: # Question 1 b)

import numpy as np
import matplotlib.pyplot as plt

def f1(x):
    return np.exp(x)

def f2(x):
    return np.exp(0.01*x)

def derivative1(x, dx, f):
    return (8*(f(x+dx)-f(x-dx))-(f(x+2*dx)-f(x-2*dx)))/(12*dx)

# Evaluating derivatives and errors
diff_approx1 = derivative1(1, np.logspace(-15, 1, num=50), f1)
diff_true1 = np.exp(1)

diff_approx2 = derivative1(1, np.logspace(-15, 1, num=50), f2)
diff_true2 = 0.01*np.exp(0.01*1)

error1 = np.abs(diff_approx1-diff_true1)
error2 = np.abs(diff_approx2 -diff_true2)

dx = np.logspace(-15, 1, num=50)
eps = 1e-16 # double point precision

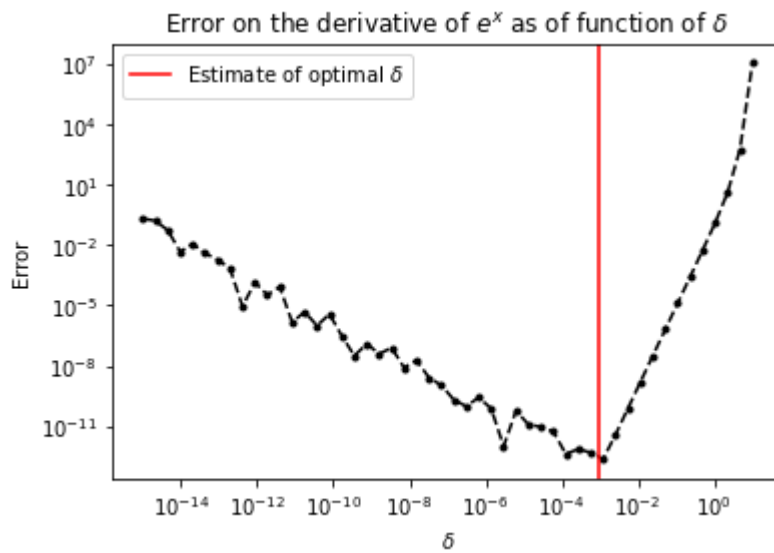
# estimate of optimal delta
delta = np.power(15*eps/2,1/5)

# Plotting stuff
plt.plot(dx, error1, 'k.--')
plt.title('Error on the derivative of $e^x$ as of function of $\delta$')
```

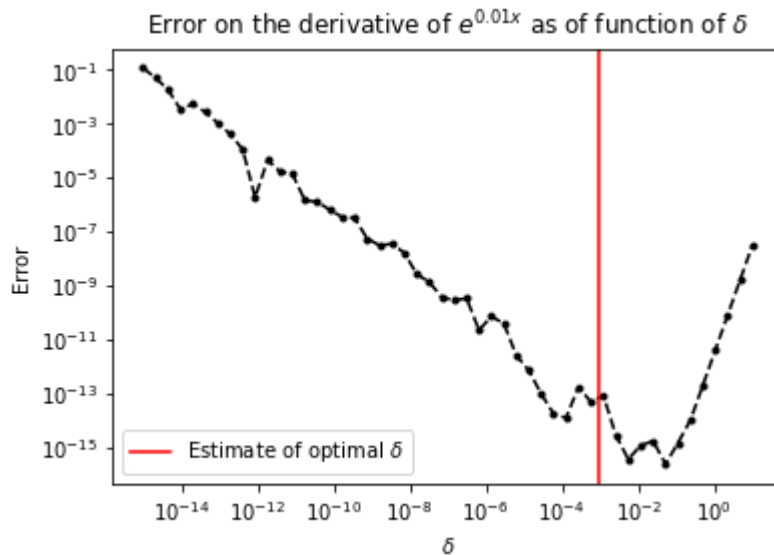
```
plt.xscale("log")
plt.yscale("log")
plt.xlabel('$\delta$')
plt.ylabel('Error')
plt.axvline(x = delta, label = 'Estimate of optimal $\delta$', color =
'r')
plt.legend()
plt.show()
print('The estimated optimal delta is', delta, '. We can see in the plot
above that it is quite close to the delta that gives us the smallest
error.')
```



```
plt.plot(dx, error2, 'k.--')
plt.title('Error on the derivative of  $e^{0.01x}$  as of function of
 $\delta$ ')
plt.xscale("log")
plt.yscale("log")
plt.xlabel('$\delta$')
plt.ylabel('Error')
plt.axvline(x = delta, label = 'Estimate of optimal $\delta$', color =
'r')
plt.legend()
plt.show()
print('The estimated optimal delta is again', delta, '. This time it is
much worse, the best delta is around 1e-1.')
print('This is because when we differentiate  $\exp(0.01x)$ , we pull down
factors of 0.01. This makes it so  $f(x)/f^{(5)}(x) = 1$  is not a good
approximation anymore.')
```



The estimated optimal delta is 0.0009440875112949016 . We can see in the plot above that it is quite close to the delta that gives us the smallest error.



The estimated optimal delta is again 0.0009440875112949016 . This time it is much worse, the best delta is around $1e-1$.

This is because when we differentiate $\exp(0.01x)$, we pull down factors of 0.01 . This makes it so $f(x)/f^{(5)}(x) = 1$ is not a good approximation anymore.

Question 2

We went through how to estimate the optimal dx for the centered derivative in class but I will reproduce it here,

$$\frac{f(x+dx) - f(x-dx)}{2dx} \approx \frac{(f(x) + dx f'(x) + \frac{1}{2} dx^2 f''(x) + \frac{1}{6} dx^3 f'''(x) + \epsilon g_1 f(x) + \dots)}{2dx}$$

This gives us

$$\frac{f(x+dx) - f(x-dx)}{2dx} \approx f'(x) + \frac{1}{6} dx^2 f'''(x) + \frac{\epsilon g f(x)}{dx}, \quad (8)$$

where I've combined g_1 and g_2 into g . The last two terms of Equation (8) are the error Δ on the derivative, so let's minimize that with respect to dx :

$$\begin{aligned}\frac{d\Delta}{d(dx)} &= \frac{1}{3}dx f'''(x) - \frac{\epsilon g f(x)}{dx^2} = 0, \\ \frac{1}{3}dx f'''(x) &= \frac{\epsilon g f(x)}{dx^2}, \\ dx &\approx \left(\frac{3\epsilon f(x)}{f'''(x)} \right)^{1/3}.\end{aligned}\tag{9}$$

The issue here is that we need to approximate the $f'''(x)$ term. I'm not sure if I was supposed to derive this here, but I looked up online an approximation scheme for the third order derivative using central difference (https://en.wikipedia.org/wiki/Finite_difference_coefficient).

$$f'''(x) = \frac{-f(x-2dx) + 2f(x-dx) - 2f(x+dx) + f(x+2dx)}{2dx}.\tag{10}$$

The idea is to use Equation (10) with some non-optimal dx to estimate the third order derivative, then use that to find the optimal dx , as well as the error Δ . There are some examples below with simple numpy functions. The code is Q2.ipynb.

```
In [ ]: # Question 2
import numpy as np
import matplotlib.pyplot as plt

def ndiff(fun, x, full = False):

    eps = 1e-16 # double digit precision
    h = 1e-16 # arbitrary, non-optimal dx

    third_derivative_estimate = (-fun(x-2*h)+2*fun(x-
h)-2*fun(x+h)+fun(x+2*h))/(2*h)

    dx = np.abs(np.cbrt((3*eps*fun(x))/third_derivative_estimate)) #
optimal dx
    err_approx = np.abs((dx**2*third_derivative_estimate)/6 +
(eps*fun(x))/dx) # error estimate

    diff_approx = (fun(x+dx)-fun(x-dx))/(2*dx) # numerical derivative
```

```

    if full == False:
        return diff_approx

    else:
        return diff_approx, dx, err_approx

# some examples with numpy functions
print('For exp(x) at x = 1, the numerical derivative is', ndiff(np.exp, 1,
full = True)[0], ', the actual value is', np.exp(1),'.')
print('The optimal dx and the error estimate are
respectively',ndiff(np.exp, 1, full = True)[1],',',ndiff(np.exp, 1, full =
True)[2],'.')
print('The real error is', np.abs( ndiff(np.exp, 1, full = True)[0]-
np.exp(1)),'.')
print('\n')
print('For sin(x) at x = 3, the numerical derivative is', ndiff(np.sin, 2,
full = True)[0], ', the actual value is', np.cos(2),'.')
print('The optimal dx and the error estimate are
respectively',ndiff(np.sin, 2, full = True)[1],',',ndiff(np.sin, 2, full =
True)[2],'.')
print('The real error is', np.abs( ndiff(np.sin, 2, full = True)[0]-
np.cos(2)),'.')
print('\n')
print('For ln(x) at x = 2, the numerical derivative is', ndiff(np.log, 2,
full = True)[0], ', the actual value is', 1/(2),'.')
print('The optimal dx and the error estimate are
respectively',ndiff(np.log, 2, full = True)[1],',',ndiff(np.log, 2, full =
True)[2],'.')
print('The real error is', np.abs( ndiff(np.log, 2, full = True)
[0]-1/(2)),'.')
print('\n')
print('We get really good numerical derivatives!')

```

For $\exp(x)$ at $x = 1$, the numerical derivative is 2.7182818284597934 , the actual value is 2.718281828459045 .
 The optimal dx and the error estimate are respectively 4.9653677458619375e-06 , 8.211723584998573e-11 .
 The real error is 7.482903185973555e-13 .

For $\sin(x)$ at $x = 3$, the numerical derivative is -0.41614683654057033 , the actual value is -0.4161468365471424 .
 The optimal dx and the error estimate are respectively 7.891307997729034e-06 , 5.761385990049813e-12 .
 The real error is 6.572076216571077e-12 .

For $\ln(x)$ at $x = 2$, the numerical derivative is 0.5000000000062907 , the actual value is 0.5 .
 The optimal dx and the error estimate are respectively 7.2086757948656255e-06 , 1.4423186732582125e-11 .
 The real error is 6.290745702131062e-12 .

We get really good numerical derivatives!

Question 3

```
In [ ]: # Question 3

import numpy as np
import matplotlib.pyplot as plt
from scipy import interpolate

data = np.loadtxt('lakeshore.txt')

def lakeshore(V, data):
    '''
    data = input data set of temperature vs voltage
    V = voltages you want to know the temperature of (between 0.090681 and
    1.644390)

    Function does a cubic spline on the data and returns the interpolated
    temperature and the estimated uncertainty
    '''

    data = data[::-1] # sort in ascending order of voltage
```



```
V_data = data[:,1]
T_data = data[:,0]

# Let's do a cubic spline using scipy

# interpolate.splrep estimates a cubic spline approximation on (x,y)
spline = interpolate.splrep(V_data,T_data)
# interpolate.splev returns the spline evaluated at the points given
T = interpolate.splev(V, spline)

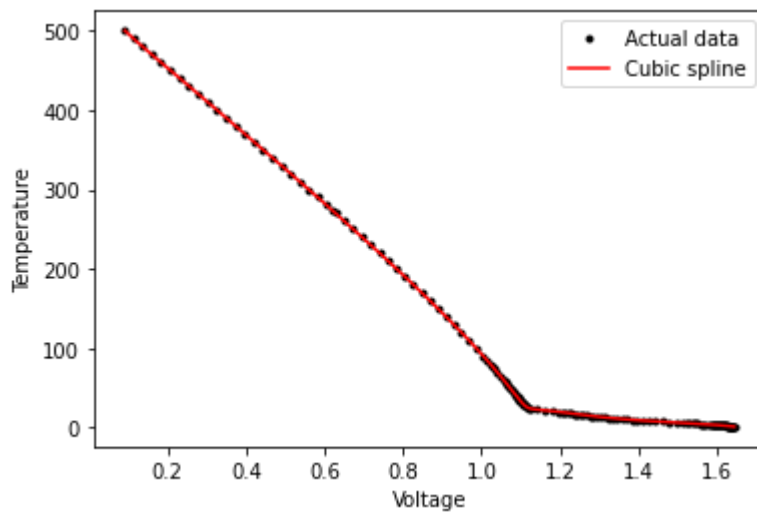
return T
```

```
In [ ]: # test of lakeshore(V, data)

test = np.loadtxt('lakeshore.txt')
test = test[:-1]
V_test = test[:,1]
T_test = test[:,0]

VV_test = np.linspace(V_test[0], V_test[-1], 2000)
test1 = test = np.loadtxt('lakeshore.txt')
TT_test = lakeshore(VV_test, test1)

plt.plot(V_test, T_test, 'k.', label = 'Actual data')
plt.plot(VV_test, TT_test, 'r', label = 'Cubic spline')
plt.xlabel('Voltage')
plt.ylabel('Temperature')
plt.legend(loc = 'best')
plt.show()
print('Doesnt look like a bad interpolation at all!')
```



Doesnt look like a bad interpolation at all!

Question 4

```
In [ ]: # Question 4
import numpy as np
import matplotlib.pyplot as plt
from scipy import interpolate

# scipy interpolation for cosine between -pi/2 and pi/2

x = np.linspace(-np.pi/2, np.pi/2, 11)
y = np.cos(x)
x_fine = np.linspace(-np.pi/2, np.pi/2, 500)

# Nearest neighbours
nearest = interpolate.interp1d(x, y, kind = 'nearest')
rmse_nearest = np.sqrt(np.mean((np.cos(x_fine) - nearest(x_fine))**2))

# Linear interpolation
linear = interpolate.interp1d(x, y, kind = 'linear')
rmse_linear = np.sqrt(np.mean((np.cos(x_fine) - linear(x_fine))**2))

# Quadratic interpolation
quadratic = interpolate.interp1d(x, y, kind = 'quadratic')
rmse_quadratic = np.sqrt(np.mean((np.cos(x_fine) - quadratic(x_fine))**2))

# Cubic spline
```

```

cubic = interpolate.interp1d(x, y, kind = 'cubic')
rmse_cubic = np.sqrt(np.mean((np.cos(x_fine) - cubic(x_fine))**2))

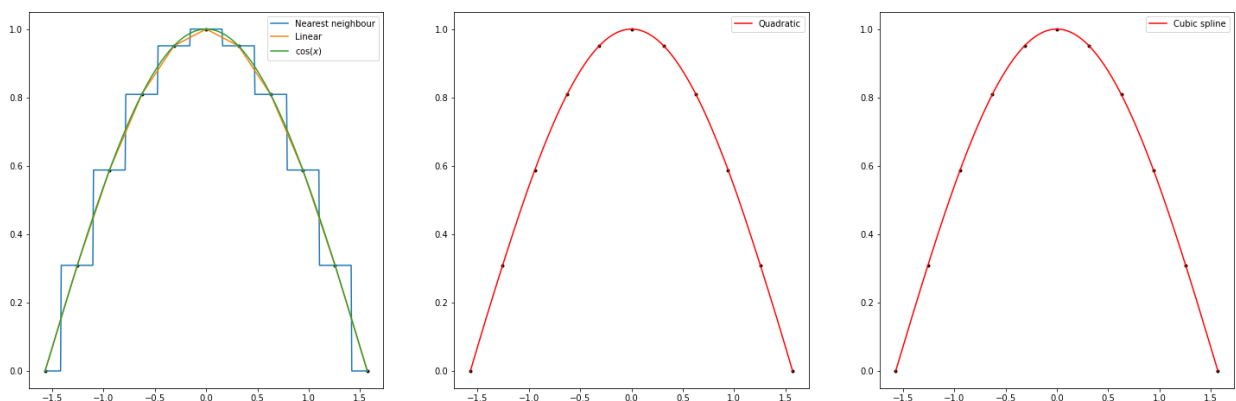
fig, ax = plt.subplots(1,3,figsize=(25,8))
ax[0].plot(x,y,'k.')
ax[0].plot(x_fine,nearest(x_fine), label = 'Nearest neighbour')
ax[0].plot(x_fine,linear(x_fine), label = 'Linear')
ax[0].plot(x_fine, np.cos(x_fine), label = '$\cos(x)$')
ax[0].legend(loc = 'best')

ax[1].plot(x,y,'k.')
ax[1].plot(x_fine,quadratic(x_fine), 'r', label = 'Quadratic')
ax[1].legend(loc = 'best')

ax[2].plot(x,y,'k.')
ax[2].plot(x_fine,cubic(x_fine), 'r', label = 'Cubic spline')
ax[2].legend(loc = 'best')
plt.show()

print("The root mean square error on the nearest neighbour interpolation
is:", rmse_nearest)
print("The root mean square error on linear interpolation is:",
rmse_linear)
print("The root mean square error on the quadratic interpolation is:",
rmse_quadratic)
print("The root mean square error on the cubic spline is", rmse_cubic)

```



The root mean square error on the nearest neighbour interpolation is: 0.0639339392182442

The root mean square error on linear interpolation is: 0.006350728317241847

The root mean square error on the quadratic interpolation is: 0.00046929553987613945

The root mean square error on the cubic spline is 3.140124235578087e-05

In []: *# Code for rational interpolation (taken from class)*

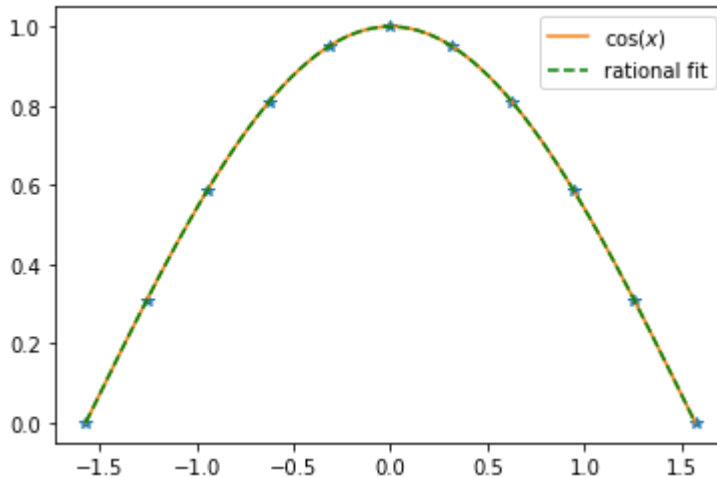
```
def rat_eval(p,q,x):
    top=0
    for i in range(len(p)):
        top=top+p[i]*x**i
    bot=1
    for i in range(len(q)):
        bot=bot+q[i]*x**(i+1)
    return top/bot

def rat_fit(x,y,n,m):
    assert(len(x)==n+m-1)
    assert(len(y)==len(x))
    mat=np.zeros([n+m-1,n+m-1])
    for i in range(n):
        mat[:,i]=x**i
    for i in range(1,m):
        mat[:,i-1+n]=-y*x**i
    pars=np.dot(np.linalg.inv(mat),y)
    p=pars[:n]
    q=pars[n:]
    return p,q

# Rat fit for cosine bewteen -pi/2 and pi/2
n=5
m=7
x=np.linspace(-np.pi/2,np.pi/2,n+m-1)
y=np.cos(x)
p,q=rat_fit(x,y,n,m)
xx=np.linspace(x[0],x[-1],500)
y_true=np.cos(xx)
pred=rat_eval(p,q,xx)
plt.clf();plt.plot(x,y,'*')
```

```
plt.plot(xx,y_true, label = '$\cos(x)$')
plt.plot(xx,pred, 'g--', label = 'rational fit')
plt.legend()
plt.show()

rmse_rat = np.sqrt(np.mean((y_true - pred)**2))
print("The root mean squared error on the rational interpolation is:",
rmse_rat)
```



The root mean squared error on the rational interpolation is: 3.3758978990759764e-09

```
In [ ]: # Scipy interpolation for a Lorentzian between -1 and 1

x = np.linspace(-1, 1, 11)

def lorentzian(x):
    return 1/(1+x**2)

y = lorentzian(x)
x_fine = np.linspace(-1, 1, 500)

# Nearest neighbours
nearest = interpolate.interp1d(x, y, kind = 'nearest')
rmse_nearest = np.sqrt(np.mean((lorentzian(x_fine) - nearest(x_fine))**2))

# Linear interpolation
linear = interpolate.interp1d(x, y, kind = 'linear')
rmse_linear = np.sqrt(np.mean((lorentzian(x_fine) - linear(x_fine))**2))
```

```
# Quadratic interpolation
quadratic = interpolate.interp1d(x, y, kind = 'quadratic')
rmse_quadratic = np.sqrt(np.mean((lorentzian(x_fine) -
quadratic(x_fine))**2))

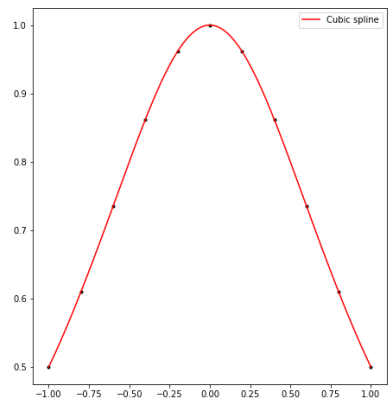
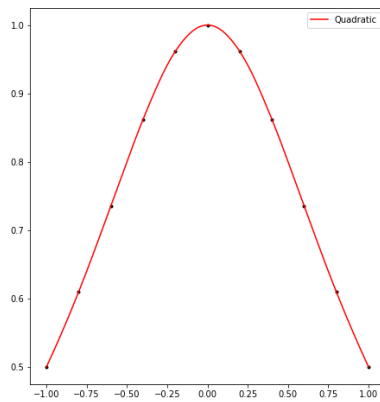
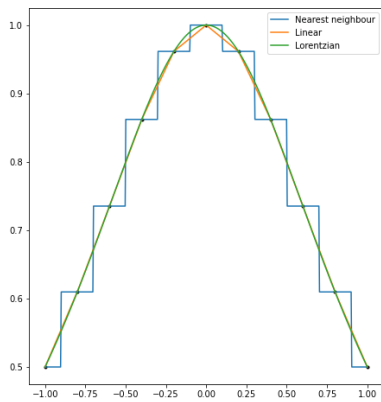
# Cubic spline
cubic = interpolate.interp1d(x, y, kind = 'cubic')
rmse_cubic = np.sqrt(np.mean((lorentzian(x_fine) - cubic(x_fine))**2))

fig, ax = plt.subplots(1,3,figsize=(25,8))
ax[0].plot(x,y,'k.')
ax[0].plot(x_fine,nearest(x_fine), label = 'Nearest neighbour')
ax[0].plot(x_fine,linear(x_fine), label = 'Linear')
ax[0].plot(x_fine, lorentzian(x_fine), label = 'Lorentzian')
ax[0].legend(loc = 'best')

ax[1].plot(x,y,'k.')
ax[1].plot(x_fine,quadratic(x_fine), 'r', label = 'Quadratic')
ax[1].legend(loc = 'best')

ax[2].plot(x,y,'k.')
ax[2].plot(x_fine,cubic(x_fine), 'r', label = 'Cubic spline')
ax[2].legend(loc = 'best')
plt.show()

print("The root mean square error on the nearest neighbour interpolation
is:", rmse_nearest)
print("The root mean square error on linear interpolation is:",
rmse_linear)
print("The root mean square error on the quadratic interpolation is:",
rmse_quadratic)
print("The root mean square error on the cubic spline is", rmse_cubic)
```



The root mean square error on the nearest neighbour interpolation is: 0.030464270246018672

The root mean square error on linear interpolation is: 0.0036913982724037374

The root mean square error on the quadratic interpolation is: 0.00018091510510278392

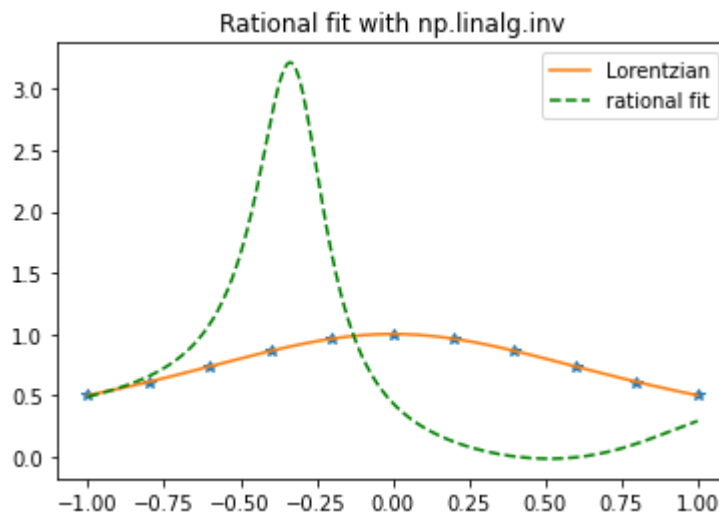
The root mean square error on the cubic spline is 0.0001125141313629842

```
In [ ]: # rational function fit on the Lorentzian

n=5
m=7
x=np.linspace(-1,1,n+m-1)
y=lorentzian(x)
p,q=rat_fit(x,y,n,m)
xx=np.linspace(x[0],x[-1],500)
y_true=lorentzian(xx)
pred=rat_eval(p,q,xx)
plt.clf();plt.plot(x,y,'*')
plt.plot(xx,y_true, label = 'Lorentzian')
plt.plot(xx,pred, 'g--', label = 'rational fit')
plt.title('Rational fit with np.linalg.inv')
plt.legend()
plt.show()

p_inv = p
q_inv = q

rmse_rat = np.sqrt(np.mean((y_true - pred)**2))
print("The root mean squared error on the rational interpolation is:",
      rmse_rat)
print('Wow that is really not good!')
```



The root mean squared error on the rational interpolation is: 0.8500774166773788
Wow that is really not good!

In []: *# Let's try using np.linalg.pinv in the rational fit*

```
def rat_fit_new(x,y,n,m):
    assert(len(x)==n+m-1)
    assert(len(y)==len(x))
    mat=np.zeros([n+m-1,n+m-1])
    for i in range(n):
        mat[:,i]=x**i
    for i in range(1,m):
        mat[:,i-1+n]=-y*x**i
    pars=np.dot(np.linalg.pinv(mat),y)
    p=pars[:n]
    q=pars[n:]
    return p,q

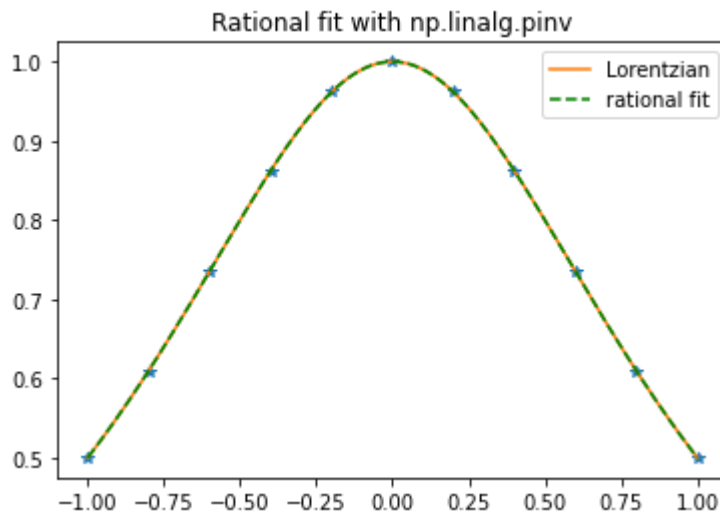
n=5
m=7
x=np.linspace(-1,1,n+m-1)
y=lorentzian(x)
p,q=rat_fit_new(x,y,n,m)
xx=np.linspace(x[0],x[-1],500)
y_true=lorentzian(xx)
pred=rat_eval(p,q,xx)
plt.clf();plt.plot(x,y,'*')
plt.plot(xx,y_true, label = 'Lorentzian')
plt.plot(xx,pred, 'g--', label = 'rational fit')
```



```
plt.title('Rational fit with np.linalg.pinv')
plt.legend()
plt.show()

p_pinv = p
q_pinv = q

rmse_rat = np.sqrt(np.mean((y_true - pred)**2))
print("The root mean squared error on the rational interpolation is:",
      rmse_rat)
print('This much better! Lets look at p and q to try and figure out what
      changed.')
print('p and q obtained from np.linalg.inv:', p_inv, q_inv)
print('p and q obtained from np.linalg.pinv:', p_pinv, q_pinv)
```



```
The root mean squared error on the rational interpolation is: 4.134146169365445e-16
This much better! Lets look at p and q to try and figure out what changed.
p and q obtained from np.linalg.inv: [ 0.43701074 -0.75      -1.        -2.
 6.        ] [ 4.25  4.   -4.    2.   -4.    6.   ]
p and q obtained from np.linalg.pinv: [ 1.00000000e+00  0.00000000e+00 -3.75000000e-0
1 -4.30211422e-16
 1.25000000e-01] [ 4.4408921e-16  6.2500000e-01  4.4408921e-16 -2.5000000e-01
 4.4408921e-16  1.2500000e-01]
```

There's an enormous difference between the p 's and q 's obtained using `np.linalg.inv` (`inv`) and `np.linalg.pinv` (`pinv`). Most of the entries obtained from `inv` are greater than 1, which is not normal, while the entries obtained from `pinv` are all less than 1, with most of them being zero. This is probably because the matrix in that case is singular (determinant is zero or close to zero), and `np.linalg.pinv` is able to handle that.