

```
In [4]: import numpy as np
from matplotlib import pyplot as plt
from scipy import interpolate as interp
from scipy import stats
import warnings; warnings.simplefilter('ignore')
```

Note that Loïc Miara and me helped each other on this assignment which can be found [here](#).

PROBLEM ONE

PROBLEM ONE

The first terms

$$f(x - \delta) = f(x) - f^1(x)\delta + \frac{1}{2}f^2(x)\delta^2 - \frac{1}{6}f^3(x)\delta^3 +$$

$$\begin{aligned} f(x+2\delta) &= f(x) + f^1(x)\delta + 2f^2(x)\delta^2 + \frac{8}{6}f^3(x)\delta^3 + \frac{16}{24}f^4(x)\delta^4 + \frac{32}{120}f^5(x)\delta^5 + \dots \\ f(x-2\delta) &= f(x) - f^1(x)\delta + 2f^2(x)\delta^2 - \frac{8}{6}f^3(x)\delta^3 + \frac{16}{24}f^4(x)\delta^4 - \frac{32}{120}f^5(x)\delta^5 + \dots \end{aligned}$$

Now, by subtracting $f(x + \delta)$ and $f(x - \delta)$, the even terms cancel out such that,

$$\frac{f(x+\delta)-f(x-\delta)}{2\delta} \approx f^1(x) + \frac{1}{6}f^3(x)\delta^2 + \frac{1}{120}f^5(x)\delta^4 + \dots \quad (1)$$

$$\frac{f(x+2\delta)-f(x-2\delta)}{4\delta} \approx 3f^1(x) + \frac{2}{3}f^3(x)\delta^2 + \frac{32}{120}f^5(x)\delta^4 + \dots \quad (2)$$

$$\frac{f(x+2\delta)-f(x-2\delta)}{4\delta} - 4\frac{f(x+\delta)-f(x-\delta)}{2\delta} = -3f'(x) + \frac{7}{30}f'''(x)\delta^4 + \dots$$

With a truncation error $\delta^4 f^5(x)$, we obtain the following numerical approximation for $f'(x)$

$$f'(x) \approx \frac{8|f(x+\delta)-f(x-\delta)|-|f(x+2\delta)-f(x-2\delta)|}{12\delta}$$

The total error is the sum of the round-off and truncation error (10^{-16}).

Set it equal to zero and differentiate with respect to δ to minimize the error:

$$\frac{f\epsilon}{\delta^2} + 4\delta^3 f^5(x) = 0 \iff -f\epsilon + 4\delta^5 f^5(x) = 0$$

$\Leftrightarrow \delta \approx (\epsilon \frac{1}{f})^{1/5} (1)$

Now, $\frac{1}{f}$ for $f(x) = e^x$ is 1 for all x and $\frac{1}{f}$ for $f(x) = e^{0.01x}$ is 10^{10} for all x . Therefore, plugging these and ϵ in (1) yields

$\delta_e \approx 10^{-3}$ and $\delta_{e^{0.01x}} \approx 10^{-1}$.

```
In [5]: #This code is inspired from John's "num_derivs_clean.py" code.

logdx=np.linspace(-8,0,1001)
dx=10**logdx #dx's range from 1e-8 to 1

fun=np.exp
x0=1 #the function is evaluated at x=1

#The four points where the function is evaluated
y1=fun(x0+dx)
y2=fun(x0-dx)
y3=fun(x0+2*dx)
y4=fun(x0-2*dx)

#Similarly, the four points evaluated for f(x) = exp(0.01x)
y1=fun(x0*dx/100)
y2=fun(x0-dx/100)
y3=fun(x0+2*dx/100)
y4=fun(x0-2*dx/100)

#The returned numerical derivatives
d1=1/(12*dx)*(8*(y1-y2)-(y3-y4)) #for f(x) = exp[x]
d2=1/(12*dx)*(8*(y1-y2)-(y3-y4)) #for f(x) = exp[0.01x]

#Compute the best dx estimation
def est_dx(ratio,n):
    return (1e-16*ratio)**n

n=1/5
ratio1=1
ratio2=1e10

dx1=est_dx(ratio1,n)
dx2=est_dx(ratio2,n)
print('The best estimated of dx for f(x)=exp[x] is ~{} \
and for f(x)=exp[0.01x], ~{}',format(round(dx1,4),round(dx2,2)))

#Plot the Figure
fig = plt.subplots(1,figsize=(12,6))
ax=plt.gca()
plt.loglog(dx,np.abs(d1-np.exp(x0)),label='$f(x) = exp(x)$',color = 'b')
plt.loglog(dx,np.abs(d2-1/100*np.exp(x0/100)),label='$f(x) = exp(0.01x)$',color = 'r')
plt.title('Derivative Errors',fontsize=16)
plt.xlabel('Delta',fontsize=15)
plt.ylabel('Error',fontsize=15)
plt.legend(loc=2, prop={'size': 16})
plt.arxline(x = dx1, linestyle='-',color = 'b')
plt.arxline(x = dx2, linestyle='--',color = 'r')
ax.set_xlim(1e-8,1)
plt.show()
```

The best

PROBLEM 2

```

In [6]: #This code is inspired from John's "num_driva_clean.py" code as well.

def ndiff(fun,x,Full=False,showPrints=True):
    try: #This try-except block is to test if the argument x is an array
        if len(x)!=0:
            #deleted the 0 element if present in the array since it could yield crasiness
            if 0 in x:
                ind=np.where(x==0)
                x = np.delete(x,ind)
                print('The element 0 at index {} has been removed from the array'.format(ind[0]))
            #notifies that 0 is removed
        except:
            if x==0:
                print('Error: The testing point cannot be zero') #Test case because this method cannot use point
                return None
            else:
                delta=1e**(1/3)*np.abs(x)
                #this is the formula to estimate the optimal dx (eq. 5.7.8 p.187 in Numerical Reciped in C, 2nd edition)
                #It is mentioned that when no information is given on the characteristic scale (i.e. (f/f')^(1/3)),
                #It is often assumed to be approximated by x (except at/near 0)

            deriv=(fun(x+dx)-fun(x-dx))/(2*dx) #centered derivative using two points

    if Full:
        fract_err=1e-16**(2/3) #Error estimation given in eq. 5.7.9 in Numerical Reciped in C, 2nd edition
        if showPrints:
            print('Derivative f'(x) = {}: dx={}: Error estimator={}'.format(deriv,dx,fract_err))
        return deriv,dx,fract_err
    else:
        if showPrints:
            print("Derivative f'(x)={}".format(deriv))
        return deriv

In [7]: #Testing the function

#Test case if a 0 is entered as the testing point
print('Test with exponential function, test point=0:')
deriv = ndiff(np.exp,0)
print('\n')

#Test case if 0 is in the array of the testing points
print('Test with exponential function, testing points contain a zero:')
deriv = ndiff(np.exp,np.linspace(0,5,11))
print('\n')

#Cosine
print('Test with cosine function:')
xx = np.linspace(-np.pi,np.pi,1001)
xx2 = np.linspace(-np.pi,np.pi,101)
print('Interval of 1001 points:')
deriv,dx,error = ndiff(fun=np.cos,xx=xx,Full=True,showPrints=False)
x_use = np.delete(xx,500)
y_true = -np.sin(x_use)
print('Interval of 101 points:')
deriv2 = ndiff(fun=np.cos,xx=xx2,showPrints=False)
y_true2 = -np.sin(xx2)

fig,axs = plt.subplots(3,figsize=(12,8),gridspec_kw={'height_ratios': [2,1,1]})
axs[0].set_title('Cosine and Numerical Derivative',fontsize=18)
axs[0].plot(x_use,deriv,label='Numerical Derivative',color='b',linestyle='solid')
axs[0].plot(x_use,y_true,label='f(x)=-sin(x)',color='r',linestyle='dashed')
axs[0].legend()
axs[1].plot(x_use,y_true-deriv,'o',markersize=2,label='Interval of 1001 points')
axs[1].set_ylabel('Errors',fontsize=12)
axs[1].legend()
axs[2].plot(x_use,y_true-deriv2,'o',markersize=2,label='Interval of 101 points')
axs[2].set_ylabel('Errors',fontsize=12)
axs[2].legend()

print('It is observed that the errors are about an order of 10 bigger for points close to zero. Nevertheless
the errors remain of ~ 1e-10. The errors of the points closer to 0 for the 101 points interval ~
remain in the order of 1e-11 as they are further away from 0.')

```

Test with exponential function, testing points contain a zero:
The element 0 at index [0] has been removed from the array
Derivative $f'(x)=[1.64872127 \quad 2.71828183 \quad 4.48168907 \quad 7.3890561 \quad 12.18249396 \quad 20.08553692 \quad 33.11545196 \quad 54.59815004 \quad 90.01713131 \quad 148.41315912]$

Test with cosine function:
Interval of 1001 points:
The element 0 at index [500] has been removed from the array
Interval of 101 points:
It is observed that the errors are about an order of 10 bigger for points closer to zero. Nevertheless, errors remain of $\sim 1e-10$. The errors of the points closer to 0 for the 101 points interval remain in order of $1e-11$ as they are further away from 0.

Cosine and Numerical Derivative

Top plot: $f(x)$ vs x . Legend: Numerical Derivative (blue line), Mean of $dx: 7.33e-06$ (orange line), Error estimate: $1e-11$ (orange line), $f(x)=\cos(x)$ (orange line).

Middle plot: Errors vs x . Legend: Interval of 1001 points (blue dots). Scale: $1e-10$.

Bottom plot: Errors vs x . Legend: Interval of 101 points (blue dots). Scale: $1e-11$.

PROBLEM 3

```
In [8]: #Download the data
data = np.loadtxt("Lakeshore.txt")

#data is flipped because scipy needs it to be ordered
voltages = np.flip(data[:,1])
temperatures = np.flip(data[:,0])

fig=plt.figure(figsize=(10,5))
plt.plot(voltages,temperatures,'o',markersize=1,
plt.xlabel("Voltage [V]",fontsize=12)
plt.ylabel("Temperature [K]",fontsize=12)
plt.title("Lakeshore Observation Data",fontsize=14)
Text(0.5, 1.0, 'Lakeshore Observation Data')
```

Lakeshore Observation Data

Temperature [K] vs Voltage [V].

I wanted to
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though that the rational interpolation would provide a good fit, but the length of the data is very long which requires very high numerator and denominator order and returns a crazy interpolation. I wondered if it would be best to try to fit for every some interval and then add the solutions but since the cubic spline provides a very good interpolation, I decided to use it to interpolate the temperatures.

```
In [9]: #Following are the fits we learned in class

#linear fit
def linear_eval(x,y,point):
    # This interpolation "draws" a linear line between each point. Then, to interpolate at a point,
    # find the two closest
    # points (a and b) are found and the returned value is interpolated from the "drawn" line between (a and b)

    # the points interpolated that are exactly = some xi value (from the data) will always have
    # the value exactly = y1
    myfun=interp.interpld(x,y,'linear')
    return myfun(point)
```

```
#Polynomial Fit
def poly_eval(x_data, y_data, n, point):

    pp=np.polyfit(x_data,y_data,n) #numpy's polynomial fitter
    #Numpy description:
    #fit a polynomial of degree n to points (x_data, y_data). Returns the coefficients p that minimises
    #the squared error in the order n, n-1, ..., 0.
    return np.polyval(pp,point) #uses the coefficients pp and evaluates the polynomial for each point

#Rational Fit
def rat_return(p,q,x):

    #These loops build the rational polynomials
    top=0
    #loop for numerator
    for i in range(len(p)):
        top+=p[i]*x**i #multiply with coefficients, sum the terms
    bot=1
    #loop for denominator
    for i in range(len(q)):
        bot+=q[i]*x**(i+1) #multiply with coefficients, sum the terms
    return top/bot #R(n) = polynomial of numerator / polynomial of denominator

def rat_eval(x,y,n,m,point):

    #This function computes the coefficients
    assert (len(x)==n+1) #checking that the sum of the orders-1 corresponds to the length of the data to
    #interpolate
    assert (len(y)==len(x))

    mat=np.zeros([n+1,n+1]) #n+1 by n+1 matrix which consists of the elements from y(x) - y(X)qq(X)
    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) #inverse the matrix and multiply the entries with y's,
#the results are p and q
p=pars[:n]
q=pars[n:]

return rat_return(p,q,point)

def eval2(x,y,n,m,point):
    #name function as above, but uses np.linalg.inv instead of np.linalg.pinv (see problem 4 for
    #comparison between the two)
    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 rat_return(p,q,point)

#Cubic Spline fit
def cubespline_eval(x,y,point):
    spln=interp.splrep(x,y) #Approximates a smooth cubic spline; returns the vector of knots,
    #the B-spline coefficients, and the degree of the spline (3 since it's cubic)
    return interp.splev(point,spln) #Evaluates the spline at the points using the vector of knots
    #and the B-spline coefficients

```

```

interp_cub = CubSpline_eval(voltages, temperatures, xx)
y_cub = cubSpline_eval(voltages, temperatures, voltages)

fig, axs = plt.subplots(4, figsize=(8,8), gridspec_kw={'height_ratios': (2,2,1,1)})
axs[0].plot(xx,interp_lin,color='g',label='Linear')
axs[0].plot(xx,interp_cub,color='b',label='Polynomial')
axs[0].plot(xx,interp_cub,color='r',label='Cubic Spline')
axs[0].legend()
axs[0].set_ylabel('Temperature [K]')
axs[0].set_title('Lakeshore Interpolation')
axs[1].plot(xx,interp_rat,label='Rational going crazy!')
axs[1].set_ylabel('Temperature [K]')
axs[1].legend()
axs[2].plot(voltages,temperatures-y_pol,'.',color='b',label='Polynomial')
axs[2].plot(voltages,temperatures-y_cub,'.',color='r',label='Cubic Spline (error ~1%)')
axs[2].format('d',np.round(np.std(np.abs(temperatures-y_cub))))))
axs[2].set_ylabel('Residual')
axs[2].set_xlabel('Voltage [V]')
axs[2].legend()
axs[3].plot(xx,interp_cub-interp_lin,'.',color='orange',label='Spline - linear')
axs[3].set_xlabel('Voltage [V]')
axs[3].set_ylabel('Residual')
axs[3].legend()

<matplotlib.legend.Legend at 0x13f057a3d>

```

The figure consists of three vertically stacked plots sharing a common x-axis representing Voltage [V] from 0.2 to 1.6.

- Top Plot:** Temperature [K] vs. Voltage [V]. The y-axis ranges from -200 to 100. A blue line shows a sharp vertical increase in temperature at approximately 1.4 V, labeled 'Rational going crazy!'.
- Middle Plot:** Residuals vs. Voltage [V]. The y-axis ranges from -2 to 2. It compares three methods: Polynomial (blue dots), Cubic Spline (red dashed line), and Error $\sim 1e-14$ (pink dots). The polynomial residuals show significant oscillations, while the cubic spline residuals are very close to zero.
- Bottom Plot:** Residuals vs. Voltage [V]. The y-axis ranges from -0.1 to 0.0. It compares the Spline - linear difference (orange line with dots). The residuals are mostly near zero, with some small spikes around 0.6 V and 1.1 V.

The text below the plots explains that linear residuals were not plotted because they would be computed as temperatures (voltages) - linearfit(voltages) which is always 0 with this type of interpolation. It notes that the cubic spline is much better than the polynomial (as expected) and that the difference between the spline and the linear fit is also pretty good, suggesting the linear fit could have been used for interpolation as well (with estimated errors $\sim 1e-13$). The cubic spline is chosen for interpolation because it provides a smooth fit.

```
def lakeshore(V,data):
    temps = np.flip(data[:,0])
    volts = np.flip(data[:,1])
```

```
#First, use the cubic spline fit
interp = CubicSpline_eval(volts, temps, V)

#Now evaluate error estimate
temps_pred = CubicSpline_eval(volts, temps, volts)
errors = np.abs(temps-temps_pred)
#asking the standard deviation of the errors to estimate the error (inspired technique from John's)
stds = 10*np.round(np.log10((np.std(errors)))) #rounding the errors to the nearest power of
#10 as they are very small

return (interp, stds)
```

In [13]:

```
#Testing the interpolation
x=0.8
xx=np.linspace(volts[0],volts[-1],1001)
test1=Lakeshore(xx,data)
test2=Lakeshore(x,data)
fig=plt.figure(figsize=(10,5))
plt.plot(volts,temperatures,'o',markersize=3,color='k',label='True values')
plt.plot(xx,test1[0],color='r',label='1001 points test')
plt.plot(x,test2[0],color='g',label='Single point test')
plt.legend()
plt.xlabel('Voltage [V]',fontsize=12)
plt.ylabel('Temperature [K]',fontsize=12)
plt.title('Lakeshore: Cubic Spline Interpolation',fontsize=14)
```

Out [13]:

Text (0.5, 1.0, 'Lakeshore: Cubic Spline Interpolation')

Temperature

Voltage [V]

PROBLEM 4

The polynomial, cubic spline and rational interpolations are already defined in a block above so I used them here too.

```
[n] [14]: n3:=3 #Rational order of n=3 and m=3, I use the order 5 for the polynomial to remain consistent.
          #5 cos points are used.

          x_points = np.linspace(-np.pi/2,np.pi/2,n+1) #5 x points
          y_points = np.cos(x_points) #cos(x) of the 5 points

          #I use an 'Marsden' (see ref. of 1003) 4 x points used to make the 5th (external) to make better
```

```
x_llcs =
#to obse
indl = n
#is from
```

```
ind2 = np.where(x_fits==np.pi/2)[0][0]
y_true = np.cos(x_fits[ind1:ind2]) #true values of the large array, used to determine the accuracy
```

```
#Polynomial Fit
y_poly = poly_eval(x_points,y_points,n,m-1,x_fits)

#Rational Fit
y_rat = rat_eval(x_points,y_points,n,m,x_fits)

#Cubic Spline Fit
y_cubspn = cubaspnline_eval(x_points,y_points,x_fits)

fig,ax=plt.subplots(2,figsize=(10,8),gridspec_kw={'height_ratios': [2,1]})
axs[0].plot(x_fits,y_poly,label='Polynomial',alpha=0.8)
axs[0].plot(x_fits,y_rat,label='Rational',alpha=0.8)
axs[0].plot(x_fits,y_cubspn,label='Cubic Spline',alpha=0.8)
axs[0].plot(x_fits,np.cos(x_fits),label='True values')
axs[0].plot(x_points,y_points,'*',label='Points used in fits')
axs[0].legend()
axs[0].set_ylabel('cos(x)')

axs[1].plot(x_fits[ind1:ind2],y_true-y_poly[ind1:ind2],label='Polynomial Fit',alpha=0.8)
axs[1].plot(x_fits[ind1:ind2],y_true-y_rat[ind1:ind2],label='Rational Fit',alpha=0.8)
axs[1].plot(x_fits[ind1:ind2],y_true-y_cubspn[ind1:ind2],label='Cubic Spline Fit',alpha=0.8)
axs[1].legend()
axs[1].set_ylabel('Errors')
axs[1].set_xlabel('x')

Text(0.5, 0, 'x')
```

Figure 14.1: Comparison of Polynomial, Rational, and Cubic Spline fits to a cosine function. The top plot shows the function values, and the bottom plot shows the errors. The Cubic Spline fit (green) is the most accurate, followed by the Rational fit (orange), and the Polynomial fit (blue) is the least accurate.

```
[15]: def lorentz(x): #Lorentz function
    return 1/(1+x**2)

x_points = np.linspace(-1,1,nm-1) #5 x points in the interval [-1,1]
y_points = np.array([lorentz(x) for x in x_points]) #Lorentz points

x_fits = np.linspace(-1,1,1001) # array used to make the interpolations
y_true = np.array([lorentz(x) for x in x_fits]) # True values

#Polynomial Fit
y_poly = poly_eval(x_points,y_points,nm-1,x_fits)

#Rational Fit
y_rat = rat_eval(x_points,y_points,n,m,x_fits)

#Cubic Spline Fit
y_cubspn = cubspline_eval(x_points,y_points,x_fits)

fig,axs = plt.subplots(3,figure=(10,8),gridspec_kw={'height_ratios': [2,1,1]})
axs[0].plot(x_fits,y_poly,label='Polynomial Fit',alpha=0.8)
axs[0].plot(x_fits,y_rat,label='Rational Fit',alpha=0.8)
axs[0].plot(x_fits,y_cubspn,label='Cubic Spline Fit',alpha=0.8)
axs[0].plot(x_points,y_points,'')
```

```

axs[0].plot(x_fits,[Lorentz(x) for x in x_fits],label='True values')
axs[0].legend()
axs[0].set_ylabel('Lorentz(x)')

axs[1].plot(x_fits,y_true-y_poly,'-',label='Polynomial Fit')
axs[1].plot(x_fits,y_true-y_rat,'-',label='Rational Fit')
axs[1].plot(x_fits,y_true-y_cubspn,'-',label='Cubic Spline Fit')
axs[1].legend()
axs[1].set_ylabel('Errors')

axs[2].plot(x_fits,y_true-y_rat,'-',label='Rational Fit')
axs[2].set_ylabel('Errors')
axs[2].set_xlabel('x')
axs[2].legend()

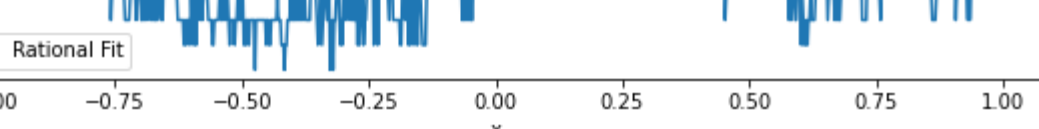
<matplotlib.legend.Legend at 0x13ac766e0>

```

The figure consists of three vertically stacked plots sharing a common x-axis ranging from -1.00 to 1.00.

- Top Plot:** The y-axis is labeled 'Lorentz(x)' and ranges from 0.5 to 1.0. It displays the 'True values' of the Lorentz function as a blue line with red dots. Three fits are overlaid: 'Polynomial Fit' (green line), 'Rational Fit' (orange line), and 'Cubic Spline Fit' (purple line). The legend is located in the top right corner.
- Middle Plot:** The y-axis is labeled 'Errors' and ranges from 0.00 to 0.02. It shows the errors for the three fits: 'Polynomial Fit' (green line), 'Rational Fit' (orange line), and 'Cubic Spline Fit' (purple line). The legend is located in the top right corner.
- Bottom Plot:** The y-axis is labeled 'Errors' and ranges from 0.00 to 2.5, with a scale factor of $1e-16$ indicated at the bottom left. It shows the errors for the 'Rational Fit' (orange line) and 'Cubic Spline Fit' (purple line). The legend is located in the top right corner.

Errors



As expected, the rational interpolation yields the best fit since a lorentzian is a rational in itself. The accuracy of the rational interpolation is indeed as good as the machine accuracy (so the error = maching rounding error)!

Increasing the orders now:

```
In [16]: #The code is similar as above

n=4;m=5 #increased order
x_points = np.linspace(-1,1,n+m-1)
y_points = np.array([lorentz(x) for x in x_points])

x_fits = np.linspace(-1,1,1001)
y_true = np.array([lorentz(x) for x in x_fits])
```

```
#Rational fit with mp.linalg.inv
y_rat1 = rat_eval(x_points,y_points,n,m,x_fits)

#Rational fit with np.linalg.inv
y_rat2 = rat_eval2(x_points,y_points,n,m,x_fits)

fig,axs = plt.subplots(1,2,figsize=(16,8))

axs[0].plot(x_fits,y_rat2,label='mp.linalg.inv')
axs[0].plot(x_fits,y_true,label='True values')
axs[0].plot(x_points,y_points,'+',label='Fitted points')
axs[0].legend()
axs[0].set_title('Lorentz Interpolation: "inv"')
axs[0].set_xlabel('x')
axs[0].set_ylabel('Lorentz(x)')

axs[1].plot(x_fits,y_rat1,label='mp.linalg.pinv')
axs[1].plot(x_fits,y_true,'-',label='True values')
axs[1].plot(x_points,y_points,'+',markersize=5,zorder=5,label='Fitted points')
axs[1].legend()
axs[1].set_title('Lorentz Interpolation: "pinv"')
axs[1].set_xlabel('x')
axs[1].set_ylabel('Lorentz(x)')

Text(0, 0.5, 'Lorentz(x)')
```

On the other hand, `np.linalg.pinv` returns the pseudo inverse by using its singular-value decomposition. This way, the rational will give an accurate interpolation of the Lorentzian, by accounting for the unexpected results that occur due to the cancelling factors

In a few words, the condition for the rational interpolation with `np.linalg.pinv` to fail is to have at least one cancelling factor (which occurs if $m > 3$ and $n > 1$).