Problem Set 2 (PHYS641) - Matias Castro Tapia

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
```

Problem 1

I defined the qrpo routine to do the least squares solution for fit parameters (for polynomial fitting) using the QR decomposition of A. Then, if $A = QR$ and we have $A^T N^{-1} Am = A^T N^{-1} d$:

$$(QR)^T N^{-1}(QR)m = (QR)^T N^{-1} d$$
$$(R^T Q^T N^{-1} QR)m = R^T Q^T N^{-1} d$$
$$m = (R^T Q^T N^{-1} QR)^{-1} R^T Q^T N^{-1} d$$
$$m = R^{-1}(Q^T N^{-1} Q)^{-1} R^{T,-1} R^T Q^T N^{-1} d$$
$$m = R^{-1}(Q^T N^{-1} Q)^{-1} Q^T N^{-1} d$$

For he specific case where $N = I$ we will have:

$$m = R^{-1}(Q^T Q)^{-1} Q^T N^{-1} d = R^{-1} Q^T N^{-1} d$$

since $Q^T Q = I$. My routine considers a general N anyway.

The routine receive x points and data $y = d$, the polynomial order o and, a noise matrix defined as the input $s = N$. The routine print the model paramaters and return the data prediction, i.e, Am.

In [2]:

```
def qrpo(x,y,o,s):
    n=len(y)
    mat=np.zeros([n,o+1])
    for i in range(o+1):
        mat[:,i]=x**i
    q,r=np.linalg.qr(mat)

    Ninv=np.linalg.inv(s)
    mod=np.linalg.inv(r)@np.linalg.inv(q.T@Ninv@q)@q.T@Ninv@y
    print(mod)
    pred=mat@mod
    return pred
```

I also defined the routine atpo for solving the least squares without the QR decomposition. Then, the solution is just $m = (A^T N^{-1} A)^{-1} A^T N^{-1} d$

In [3]:

```
def atpo(x,y,o,s):
    n=len(y)
    mat=np.zeros([n,o+1])
    for i in range(o+1):
        mat[:,i]=x**i

    Ninv=np.linalg.inv(s)
    mod=np.linalg.inv(mat.T@Ninv@mat)@mat.T@Ninv@y
    print(mod)
    pred=mat@mod
    return pred
```

Let's do a fit for $f(x) = \sin x \cos x$.

In [4]:

```
x=np.linspace(-3,3,301)
```

In [5]:

```
y1=np.sin(x)*np.cos(x)
```

I defined a noise matrix as an identity matrix.

In [6]:

```
n=len(x)
N=np.zeros([n,n])
for i in range(n):
    N[i][i]=1
```

A 22^{th} order polynomial fit using both methods.

In [7]:

```
y1predq=qrpo(x,y1,22,N)
```

```
[ 4.01940850e-16  1.00000000e+00 -6.18342183e-15 -6.66666667e-01
  2.31498848e-14  1.33333333e-01 -4.33091063e-14 -1.26984121e-02
  3.95100619e-14  7.05466894e-04 -2.18280255e-14 -2.56531355e-05
  7.54691448e-15  6.57711246e-07 -1.64717415e-15 -1.25158437e-08
  2.31504269e-16  1.82533983e-10 -2.02201588e-17 -2.01367224e-12
  1.00572258e-18  1.36829224e-14 -2.14070207e-20]
```

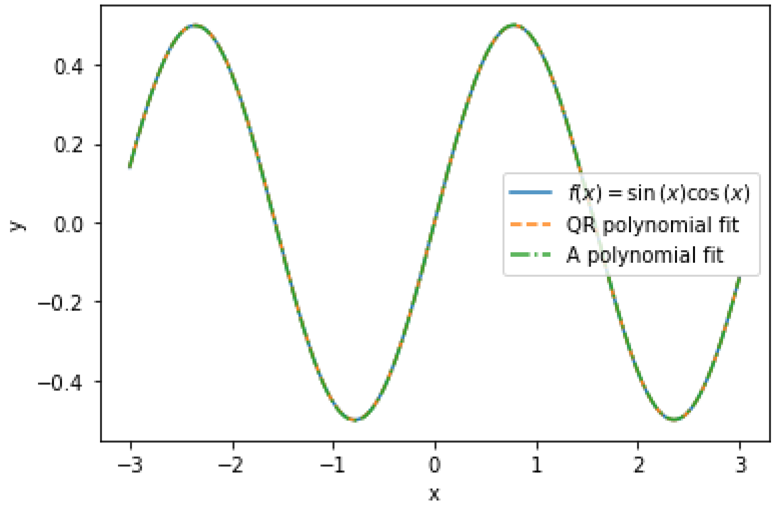
In [8]:

```
y1preda=atpo(x,y1,22,N)
```

```
[-2.77041326e-04  1.00204414e+00  1.70631879e-04 -6.67263895e-01
 -4.26173355e-05  1.33472485e-01  9.13443838e-06 -1.27162315e-02
 -4.92405347e-06  7.01804660e-04  2.41763747e-06 -2.36882014e-05
 -7.51280407e-07  2.22403810e-07  1.50679239e-07  4.85946147e-08
 -1.95582349e-08 -5.20424665e-09  1.58368688e-09  2.65643865e-10
 -7.26439171e-11 -5.69363998e-12  1.44354489e-12]
```

In [9]:

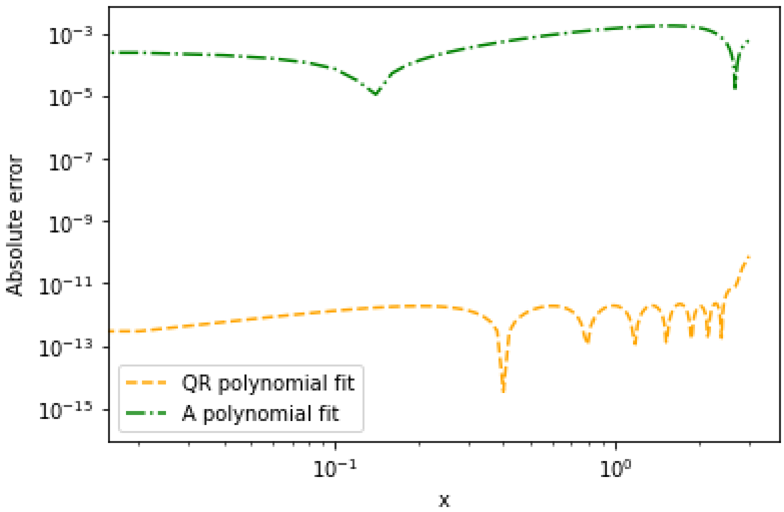
```
plt.plot(x,y1,label='$f(x)=\sin{(x)} \cos{(x)}$')
plt.plot(x,y1predq,'--',label='QR polynomial fit')
plt.plot(x,y1preda,'-.',label='A polynomial fit')
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.show()
```



It seems like both fits are very close to the function, so let's the absolute error:

In [10]:

```
plt.loglog(x,np.abs(y1predq-y1),'--',label='QR polynomial fit',color='orange')
plt.loglog(x,np.abs(y1preda-y1),'-.',label='A polynomial fit',color='green')
plt.xlabel('x')
plt.ylabel('Absolute error')
plt.legend()
plt.show()
```



Then, the absolute error is much smaller when using the QR decomposition.

Problem 2

I defined the routine Tn_fit to do a Chebyshev polynomial fit for a set of points x, data y, and order od. I used the Chebyshev polynomial definition $T_n = \cos(n \arccos(x))$ for generating the n^{th} order polynomial. Then, the i^{th} row of the matrix A for the model must be $(T_0(x_i)\ T_1(x_i)\ldots T_{od}(x_i))$ with x_i the i^{th} point. To the least squares fit for the coefficients I just used the classic linear solution $m = (A^T N^{-1} A)^{-1} A^T N^{-1} d = (A^T A)^{-1} A^T d$ (ignoring the noise matrix) . The routine returns the prediction Am and the set of coefficients m.

In [11]:

```
def Tn_fit(x,y,od):
    n=len(x)
    mat=np.zeros([n,od+1])
    for i in range(od+1):
        mat[:,i]=np.cos(i*np.arccos(x))

    mod=np.linalg.inv(mat.T@mat)@mat.T@y

    pred=mat@mod
    return pred,mod
```

I also defined the routine Tn_eval to eval an array of x points to a model coefficients as:

$$y = m_0 T_0(x) + m_1 T_1(x) + \ldots + m_{od} T_{od}(x)$$

where od=lenght of m.

In [12]:

```
def Tn_eval(x,m):
    ev=[]
    for i in range(len(m)):
        ev.append(m[i]*np.cos(i*np.arccos(x)))
    return np.array(sum(ev))
```

Let's take the xx array for the fit to e^x

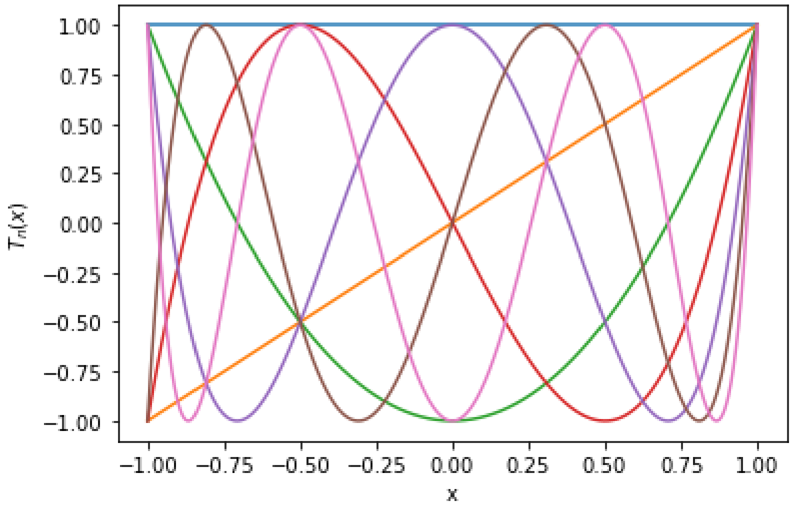
In [13]:

```
xx=np.linspace(-1,1,1000)
```

Just checking that $T_n = \cos(n \arccos(x))$ works and that they are polynomials.

In [14]:

```
for i in range(7):
    plt.plot(xx,np.cos(i*np.arccos(xx)))
plt.xlabel('x')
plt.ylabel('$T_{n}(x)$')
#plt.legend()
plt.show()
```



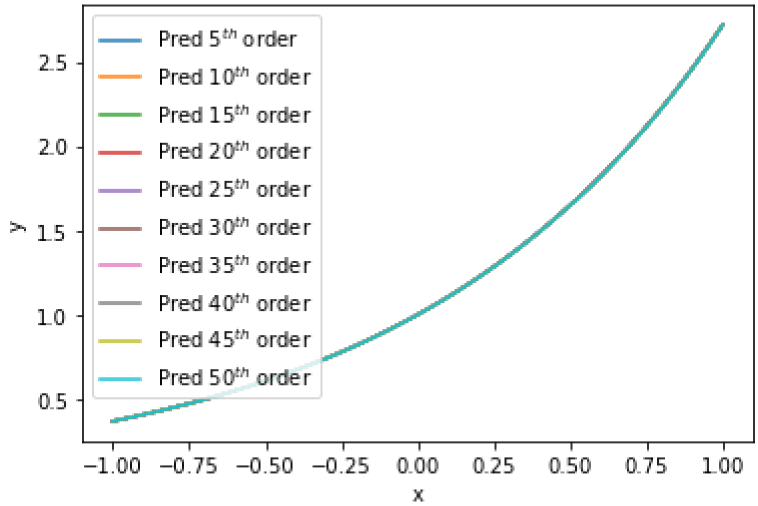
In [15]:

```
yy=np.exp(xx)
```

Let's check the stability of the fit.

In [16]:

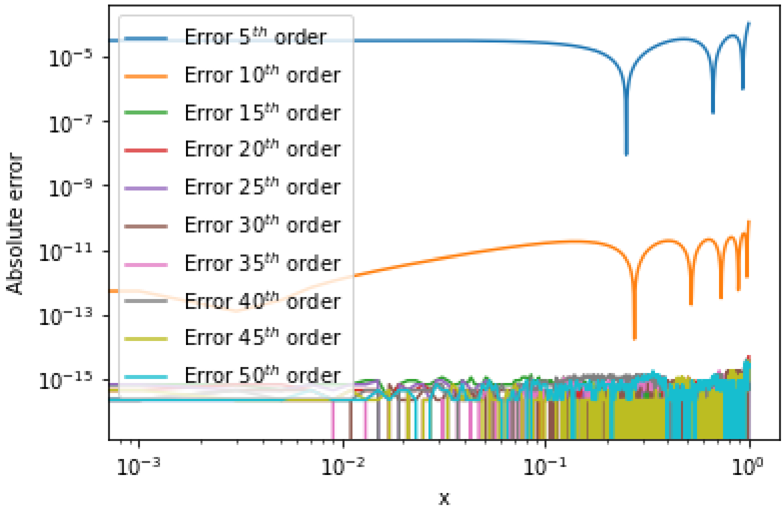
```
for i in range(5,55,5):
    predt,c=Tn_fit(xx,yy,i)
    plt.plot(xx,predt,label='Pred '+str(i)+'$^{th}$ order')
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.show()
```



It seems like it remains very stable even for a 50^{th} order fitting. So, we should look the absolute errors too.

In [17]:

```
for i in range(5,55,5):
    predt,c=Tn_fit(xx,yy,i)
    plt.loglog(xx,np.abs(yy-predt),label='Error '+str(i)+'$^{th}$ order')
plt.xlabel('x')
plt.ylabel('Absolute error')
plt.legend()
plt.show()
```



The error remains near 10^{-15} from about the 15^{th} order. Let's do a 6^{th} and a 30^{th} order fit for part b).

In [18]:

```
tn6,c6=Tn_fit(xx,yy,6)
print(c6)
```

```
[1.26606584e+00 1.13031696e+00 2.71495266e-01 4.43354952e-02
 5.47415863e-03 5.41243732e-04 4.48739566e-05]
```

In [19]:

```
maxe6=np.max(np.abs(tn6-yy))
rms6=np.sqrt(sum(np.abs(tn6-yy)**2)/len(yy))
```

In [20]:

```
print('Max error for 6th order: '+str(maxe6))
print('RMS error for 6th order: '+str(rms6))
```

```
Max error for 6th order: 7.98480781183386e-06
RMS error for 6th order: 1.9852969888235997e-06
```

In [21]:

```
tn30,c30=Tn_fit(xx,yy,30)
print(c30)
```

```
[ 1.26606588e+00  1.13031821e+00  2.71495340e-01  4.43368498e-02
  5.47424044e-03  5.42926312e-04  4.49773230e-05  3.19843646e-06
  1.99212481e-07  1.10367713e-08  5.50589491e-10  2.49789842e-11
  1.03899528e-12  3.93574062e-14  1.32532874e-15 -1.73472348e-16
 -3.46944695e-18 -1.52655666e-16 -4.16333634e-17 -2.49800181e-16
  1.17961196e-16 -7.63278329e-17 -3.46944695e-18  1.04083409e-16
  4.51028104e-17 -3.81639165e-17  6.59194921e-17 -9.02056208e-17
  1.24900090e-16 -1.42247325e-16  3.29597460e-17]
```

Now, I have to truncate the 30^{th} order fit to 6^{th}, and evaluate the truncated fit using Tn_eval

In [22]:

```
c30[7:]=0
print(c30)
```

```
[1.26606588e+00 1.13031821e+00 2.71495340e-01 4.43368498e-02
 5.47424044e-03 5.42926312e-04 4.49773230e-05 0.00000000e+00
 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
 0.00000000e+00 0.00000000e+00 0.00000000e+00]
```

In [23]:

```
tn30tr=Tn_eval(xx,c30)
```

In [24]:

```
maxe30t=np.max(np.abs(tn30tr-yy))
rms30t=np.sqrt(sum(np.abs(tn30tr-yy)**2)/len(yy))
```

In [25]:

```
print('Max error for 30th order truncated fit: '+str(maxe30t))
print('RMS error for 30th order truncated fit: '+str(rms30t))
```

```
Max error for 30th order truncated fit: 3.4092623653059206e-06
RMS error for 30th order truncated fit: 2.2588113160560264e-06
```

In [26]:

```
maxe6/maxe30t,rms6/rms30t
```

Out[26]:

```
(2.342092498685523, 0.8789122733323323)
```

If we look the old coefficients of the 30^{th} order fit (c30 before truncanting), we can note that the 8^{th} coefficient is very similar to the Max error on the truncated 30^{th} order fit, both are about 3×10^{-6}.

On the other hand, when comparing the max error for the 6^{th} order fit and the truncated 30^{th} order, we can see that it was reduced by a factor of ~ 2.3 when we truncated, while the RMS error is larger for about 14%.

Problem 3

We can start with the Cholesky decomposition of a noise matrix, then $N = LL^T$. If we consider the eigendecomposition of the matrix $N = V\Lambda V^T$ and remember that if we know $N = LL^T$ and the errors are correlated we can go from correlated data to uncorrelated as follows:

$$d_{uncorr} = L^{-1} d_{corr}$$

Thus, we can consider that $L = V\Lambda^{1/2}$ for positive eigenvalues (because N is a positive defined matrix) based on the two type of decomposition dicussed and we can obtain correlated data from uncorrelated data using the eigenvalues/vectors:

$$d_{corr} = Ld_{uncorr} = V\Lambda^{1/2} d_{uncorr}$$

I defined the routine correlated_data to generate random correlated data from an input of a noise matrix of correlated errors. The routine generates a set of random values (consistent with the length of the noise matrix) and find the eigenvalues/vectors of the noise matrix using numpy.linalg.eig. Then, it generates correlated data using $d_{corr} = V\Lambda^{1/2} d_{uncorr}$ and returns it along with $< d_{corr} d_{corr}^T >$.

$V = [\vec{v_1}\ \vec{v_2} \ldots \vec{v_n}]$ for $\vec{v_i}$ every eigenvector as a column and the element $\Lambda_{ii} = \lambda_i$ and 0 for non-diagonal elements for every eigenvalue λ_i.

In [27]:

```
def correlated_data(Ncorr):
    n=len(Ncorr)
    d=np.random.randn(len(Ncorr))

    l,vec=np.linalg.eig(Ncorr)

    lam_1=np.zeros([n,n])
    for i in range(n):
        lam_1[i][i]=l[i]

    dcorr=vec@np.sqrt(lam_1)@d

    return dcorr,np.transpose([dcorr])@[dcorr]
```

I created a matrix $N_{ij} = 1 + \delta_{ij}$ of dimensions 5×5

In [28]:

```
Ncorr=np.ones([5,5])
for i in range(len(Ncorr)):
    Ncorr[i][i]=2
```

In [29]:

```
Ncorr
```

Out[29]:

```
array([[2., 1., 1., 1., 1.],
       [1., 2., 1., 1., 1.],
       [1., 1., 2., 1., 1.],
       [1., 1., 1., 2., 1.],
       [1., 1., 1., 1., 2.]])
```

I used the routine 100 times to obtain the average of the matrix $< d_{corr} d_{corr}^T >$ for these 100 iterations.

In [30]:

```
dc100=[]
ddt100=[]
for i in range(100):
    dc,ddt=correlated_data(Ncorr)
    dc100.append(dc)
    ddt100.append(ddt)
```

In [31]:

```
sum(ddt100)/100
```

Out[31]:

```
array([[2.72615432, 1.09263198, 1.60634134, 1.3019616 , 1.69560458],
       [1.09263198, 2.57453737, 1.11429005, 1.28721382, 0.95478667],
       [1.60634134, 1.11429005, 2.26958561, 1.4525458 , 1.45165529],
       [1.3019616 , 1.28721382, 1.4525458 , 1.76675411, 1.40441788],
       [1.69560458, 0.95478667, 1.45165529, 1.40441788, 2.12578387]])
```

Now for 10000 iterations:

In [32]:

```
dc10000=[]
ddt10000=[]
for i in range(10000):
    dc,ddt=correlated_data(Ncorr)
    dc10000.append(dc)
    ddt10000.append(ddt)
```

In [33]:

```
sum(ddt10000)/10000
```

Out[33]:

```
array([[2.06883928, 0.75486194, 1.08752121, 0.93277717, 1.18082445],
       [0.75486194, 2.37963373, 0.93391176, 1.33569191, 0.68050593],
       [1.08752121, 0.93391176, 1.91416198, 1.11806224, 1.01789104],
       [0.93277717, 1.33569191, 1.11806224, 1.5830557 , 1.0546415 ],
       [1.18082445, 0.68050593, 1.01789104, 1.0546415 , 2.11083216]])
```

And 100000:

In [34]:

```
dc100000=[]
ddt100000=[]
for i in range(100000):
    dc,ddt=correlated_data(Ncorr)
    dc100000.append(dc)
    ddt100000.append(ddt)
```

In [35]:

```
sum(ddt100000)/100000
```

Out[35]:

```
array([[2.08437291, 0.75298867, 1.09358325, 0.94062985, 1.1803205 ],
       [0.75298867, 2.36025524, 0.91026667, 1.32259239, 0.67918843],
       [1.09358325, 0.91026667, 1.90795448, 1.11370475, 1.0218473 ],
       [0.94062985, 1.32259239, 1.11370475, 1.59607475, 1.06773362],
       [1.1803205 , 0.67918843, 1.0218473 , 1.06773362, 2.10052975]])
```

We can note that the average for many realizations $< d_{corr} d_{corr}^T >\sim N$

Problem 4

I defined the routine corr_noise to generate the correlated noise matrix $N_{ij} = a\exp(\frac{-(i-j)^2}{2\sigma^2}) + (1-a)\delta_{ij}$ with a, $s = \sigma$, and x as inputs. x is just used to now the length of the matrix.

In [36]:

```
def corr_noise(x,a,s):
    n=len(x)
    N=np.zeros([n,n])
    for i in range(n):
        for j in range(n):
            if i==j:
                N[i][j]=a*np.exp(-((i-j)**2)/(2*(s**2)))+(1-a)
            else:
                N[i][j]=a*np.exp(-((i-j)**2)/(2*(s**2)))
    return N
```

In [37]:

```
xs=np.linspace(0,999,1000)
```

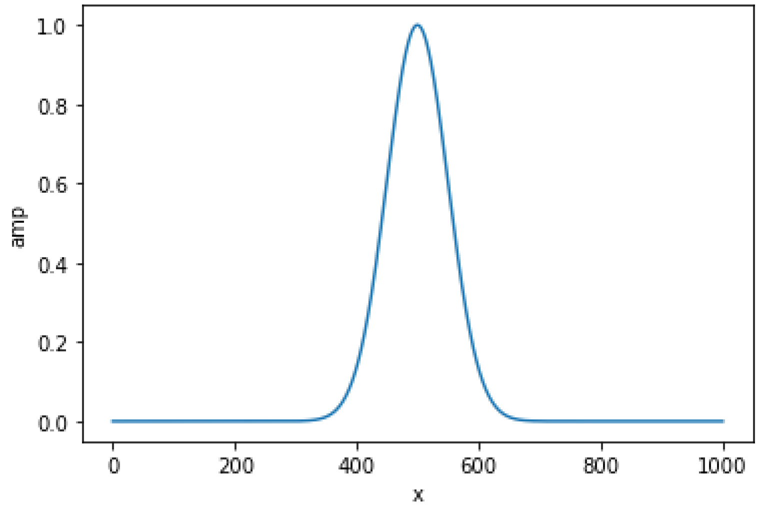
I defined the Gaussian signal for the x points.

In [38]:

```
signal=np.exp(-((xs-xs[499])**2)/(2*(50**2)))
```

In [39]:

```
plt.plot(xs,signal)
plt.xlabel('x')
plt.ylabel('amp')
#plt.legend()
plt.show()
```



I computed the error bar for the fit amplitude for each pair of a and σ using the output of the routine corr_noise. The estimation of the error bar is obtained as $\sqrt{(A^T N^{-1} A)^{-1}}$, with A the template signal and N the matrix of correlated noise.

In [40]:

```
a=[0.1,0.5,0.9]
sigma=[5,50,500]
for i in a:
    for j in sigma:
        error=np.sqrt(1/(signal@np.linalg.inv(corr_noise(xs,i,j))@signal))
        print('For a='+str(i)+' and sigma='+str(j)+
             ' the error bar on the fit is:'+str(error))
```

```
For a=0.1 and sigma=5 the error bar on the fit is:0.15576335487646098
For a=0.1 and sigma=50 the error bar on the fit is:0.3377448956231588
For a=0.1 and sigma=500 the error bar on the fit is:0.12757498758982014
For a=0.5 and sigma=5 the error bar on the fit is:0.27599935080333926
For a=0.5 and sigma=50 the error bar on the fit is:0.7140544770562327
For a=0.5 and sigma=500 the error bar on the fit is:0.10066392140726646
For a=0.9 and sigma=5 the error bar on the fit is:0.3578952599636376
For a=0.9 and sigma=50 the error bar on the fit is:0.9499319468584407
For a=0.9 and sigma=500 the error bar on the fit is:0.04892549466815368
```

The best error was for the case of $a = 0.9$ and $\sigma = 500$ where the data must be correlated over large distances but almost perfectly correlated; the error bar was 0.0489. The worst case was $a = 0.9$ and $\sigma = 50$ where the error bar was 0.9499, in this case a and σ are very closed to the amplitude and σ_{src} values, then probably when stimating $\sqrt{(A^T N^{-1} A)^{-1}}$, the coupling of the source signal and the errors could cause that the error bars will be of the order of the amplitude. The second worst was $a = 0.5$ and $\sigma = 50$ where the error bar was 0.714, that also has $\sigma = \sigma_{src}$.