# Curve fitting

August 14, 2018

## 1 Fitting relaxometry data

Let's start by looking at data from one of the given files

```
In [1]: %pylab inline
```

```
Populating the interactive namespace from numpy and matplotlib
```

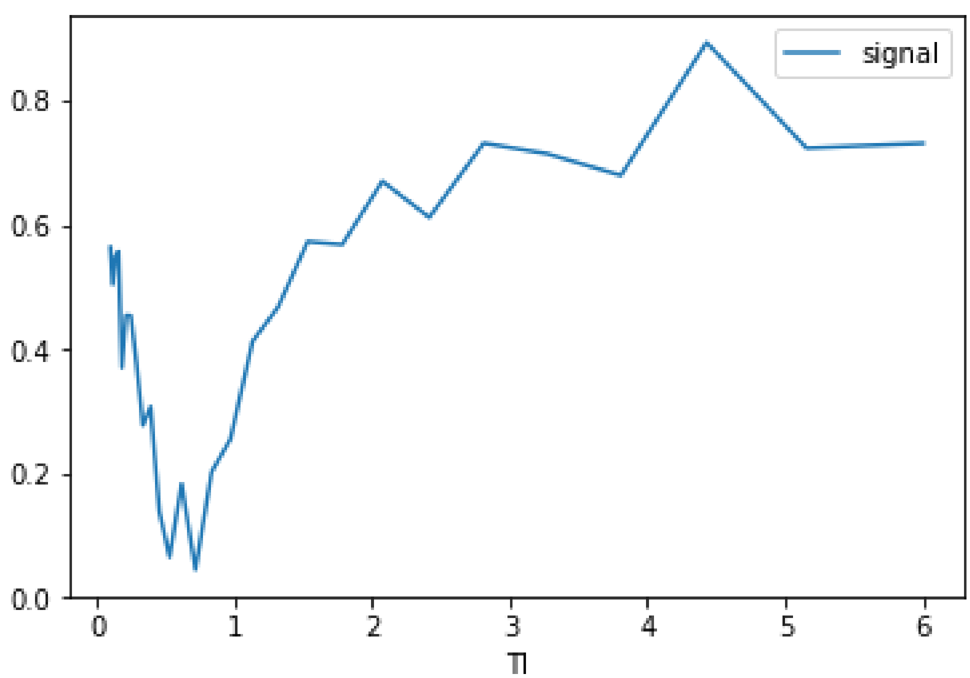
```
In [2]: import pandas as pd
```

```
/home/carlosm/venvs/py3/lib/python3.6/importlib/_bootstrap.py:219: RuntimeWarning: numpy.dtype
  return f(*args, **kwds)
```

```
In [3]: group = pd.read_csv('./data/sample.csv', index_col='TI')
```

```
In [4]: group.plot()
```

```
Out[4]: <matplotlib.axes._subplots.AxesSubplot at 0x7f274c78ecc0>
```

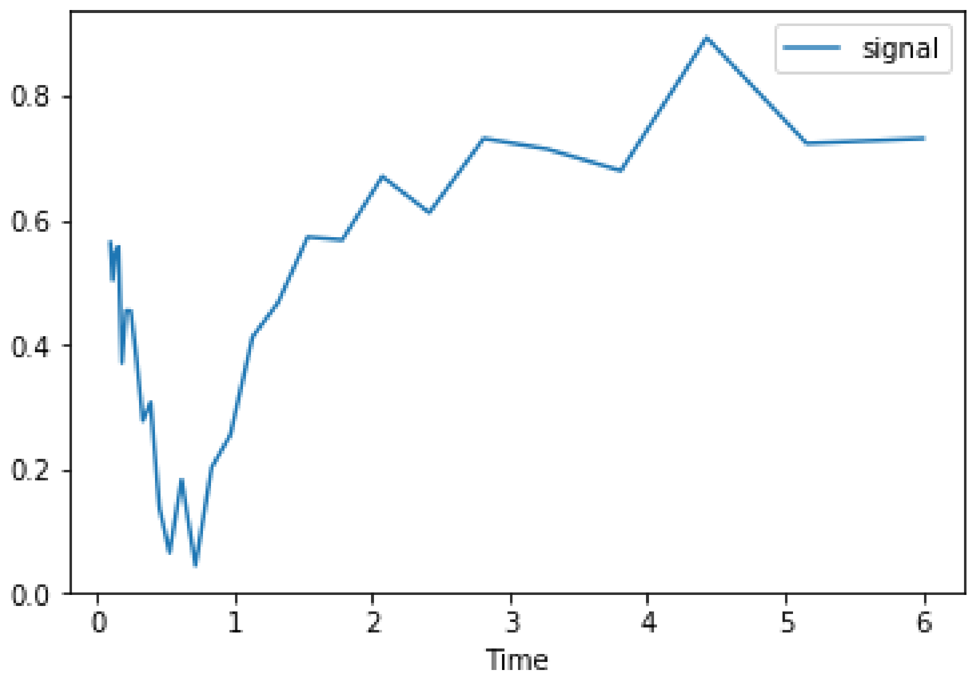


```
In [5]: groupArray = group.reset_index().values
```

```
In [6]: time = groupArray[:,0]
        signal = groupArray[:,1]
```

```
In [7]: plot(time, signal, label='signal')
        xlabel('Time')
        legend()
```

```
Out[7]: <matplotlib.legend.Legend at 0x7f2749e09c88>
```




## 2 Parameter estimation

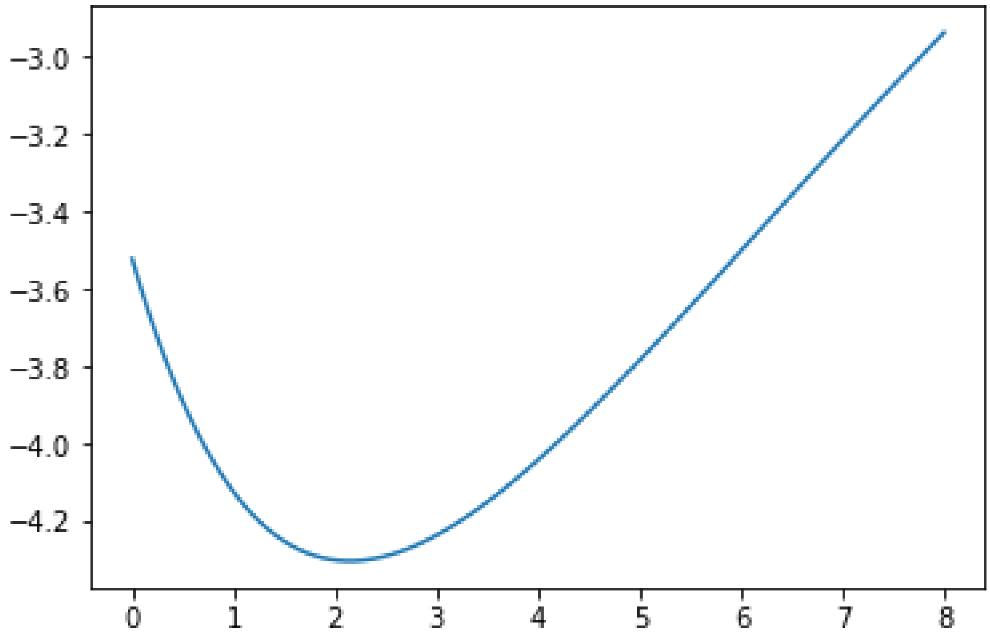
Let's build some perfect synthetic data

```
In [8]: def modelFunction(a, b, time):
            return a * np.exp(-time / 2) - b * np.exp(-(time - 0.1) / 10.)

        nSamples = 100
        t = np.linspace(0, 8, nSamples)
        # t = np.logspace(np.log(0.0001), np.log(8), nSamples)
```

```
a = np.pi
b = np.pi * 2.1
true_signal = modelFunction(a, b, t)
plot(t,true_signal)
```

Out[8]: [<matplotlib.lines.Line2D at 0x7f2749d77588>]

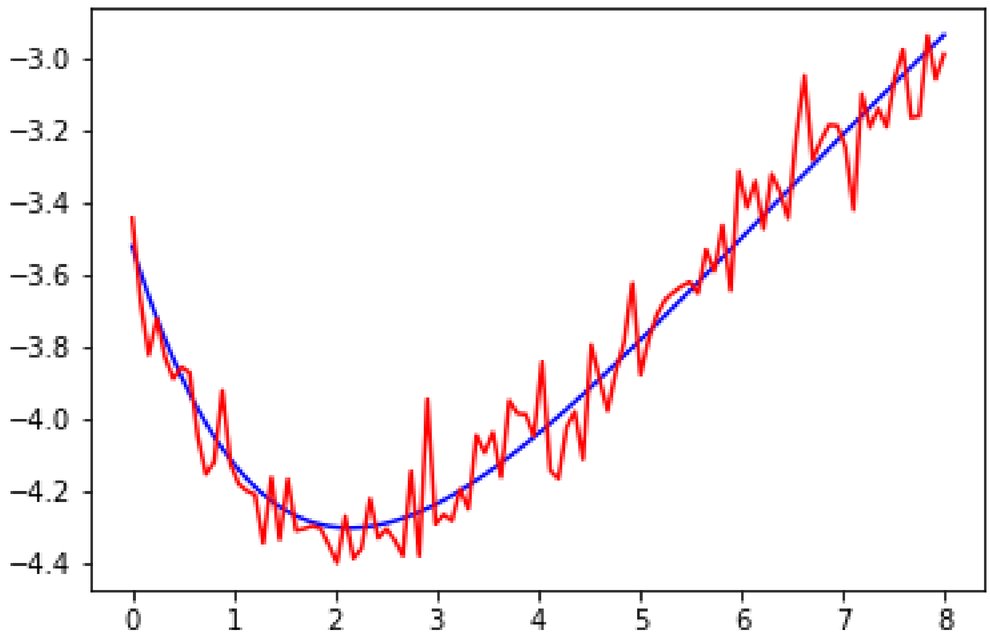



In [9]:
```
from scipy.stats import norm
```

In [10]:
```
noise = norm.rvs(loc=0, scale=0.1, size=nSamples)
noisy_signal = true_signal + noise

plot(t, true_signal, 'b-')
plot(t, noisy_signal, 'r-')
```

Out[10]: [<matplotlib.lines.Line2D at 0x7f2723bcd550>]




## 3 Let's find parameters which fit our data

Solve using `scipy.linalg.lstsq` or for `numpy.linalg.lstsq` or `lmfit`

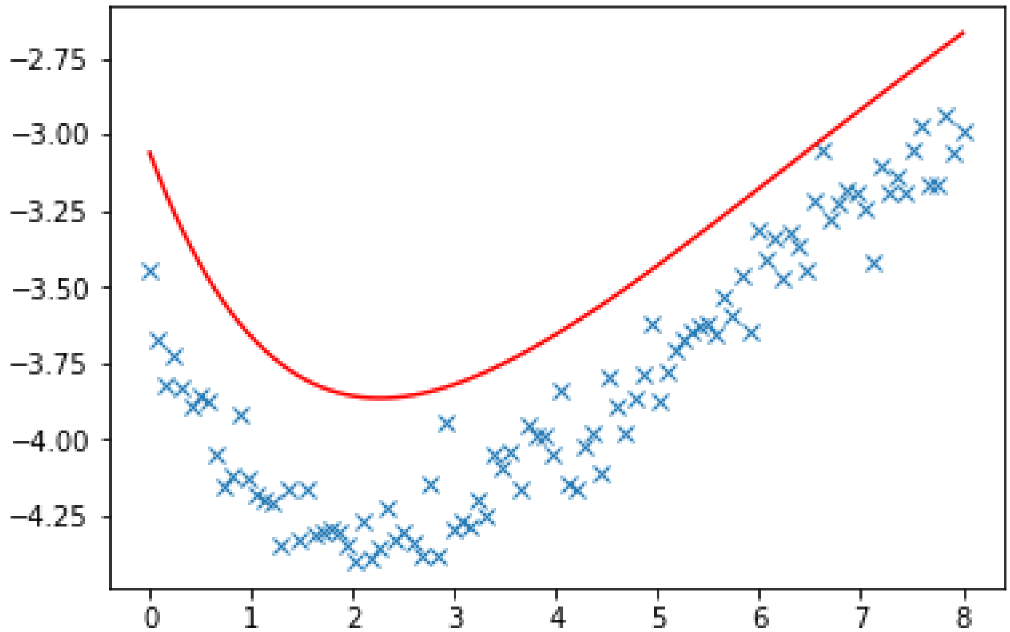
```
In [11]: # Naive method -- trial and error

         shift_guess = 3
         freq_guess = 6

         guessed_signal = modelFunction(shift_guess, freq_guess, t)

         plot(t, noisy_signal, 'x')
         plot(t, guessed_signal, 'r-')

Out[11]: [<matplotlib.lines.Line2D at 0x7f2723b99048>]
```




We can do better than manually fitting our parameters

```
In [12]: import lmfit # https://lmfit.github.io/lmfit-py/

In [13]: def errorFunction(signal, target_signal):
             return abs(target_signal - signal)

In [14]: def costFunction(params, t, target_signal):
             a = params['a'].value
             b = params['b'].value

             signal = modelFunction(a, b, t)

             return errorFunction(signal, target_signal)

In [15]: fitParams = lmfit.Parameters()
         fitParams.add('a', min=0, max=10, value=5)
         fitParams.add('b', min=0, max=10, value=5)

In [16]: result = lmfit.minimize(costFunction, fitParams, args=(t, noisy_signal))

         print('a = %.4f'%result.params['a'].value,'(ground truth = %.2f)'%a)
         print('b = %.4f'%result.params['b'].value,'(ground truth = %.2f)'%b)

a = 3.0722 (ground truth = 3.14)
b = 6.5748 (ground truth = 6.60)
```

```
In [17]: lmfit.report_fit(result.params)
```

```
[[Variables]]
    a:  3.07221571 +/- 0.04772684 (1.55%) (init = 5)
    b:  6.57476002 +/- 0.02398398 (0.36%) (init = 5)
[[Correlations]] (unreported correlations are < 0.100)
    C(a, b) =  0.826
```

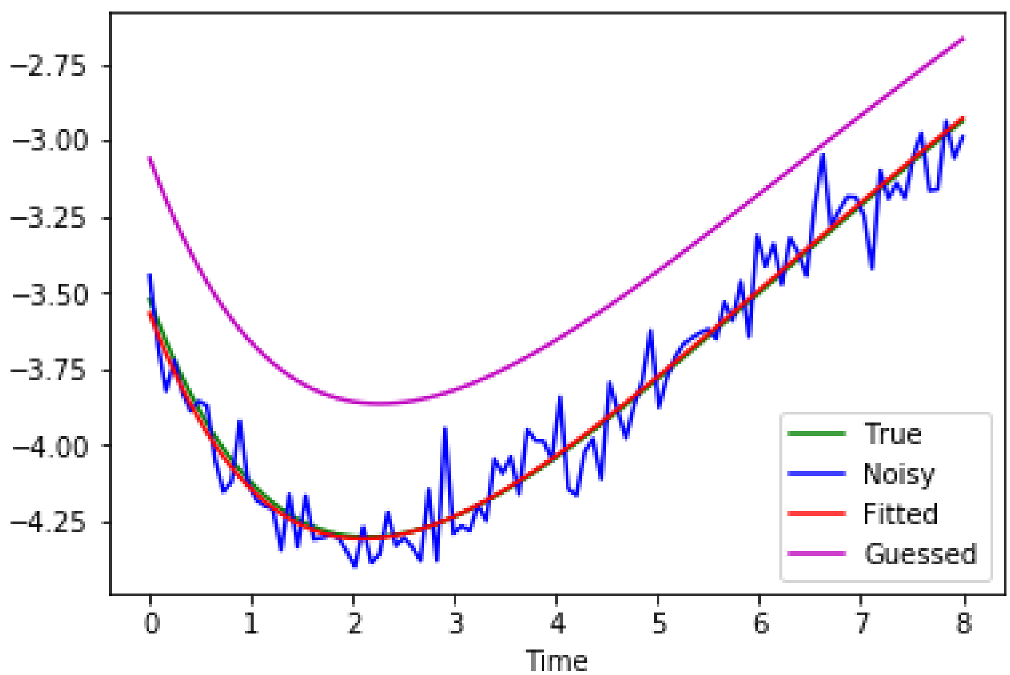
```
In [18]: a = result.params['a']
         b = result.params['b']

         fitted_signal = modelFunction(a, b, t)

         plot(t, true_signal   , 'g-', label='True')
         plot(t, noisy_signal  , 'b-', label='Noisy')
         plot(t, fitted_signal, 'r-', label='Fitted')
         plot(t, guessed_signal, 'm-', label='Guessed')

         xlabel('Time')
         legend()
```

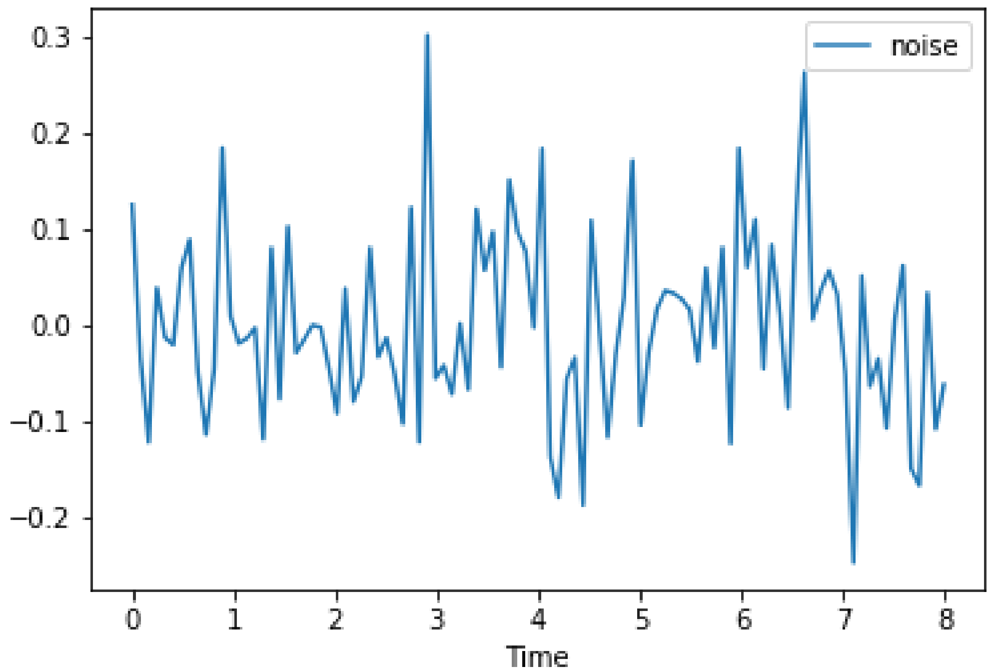
```
Out[18]: <matplotlib.legend.Legend at 0x7f2721a19358>
```



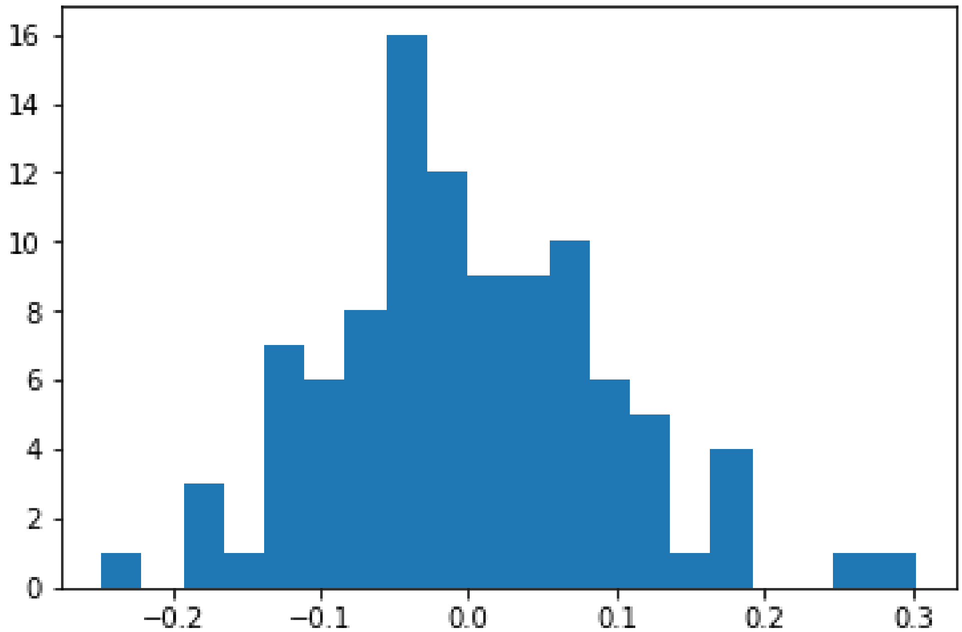
## 4 Quick look at the noise

```
In [19]: error = noisy_signal - fitted_signal
         plot(t,error, label='noise')
         xlabel('Time')
         legend()
```

```
Out[19]: <matplotlib.legend.Legend at 0x7f272198cc50>
```



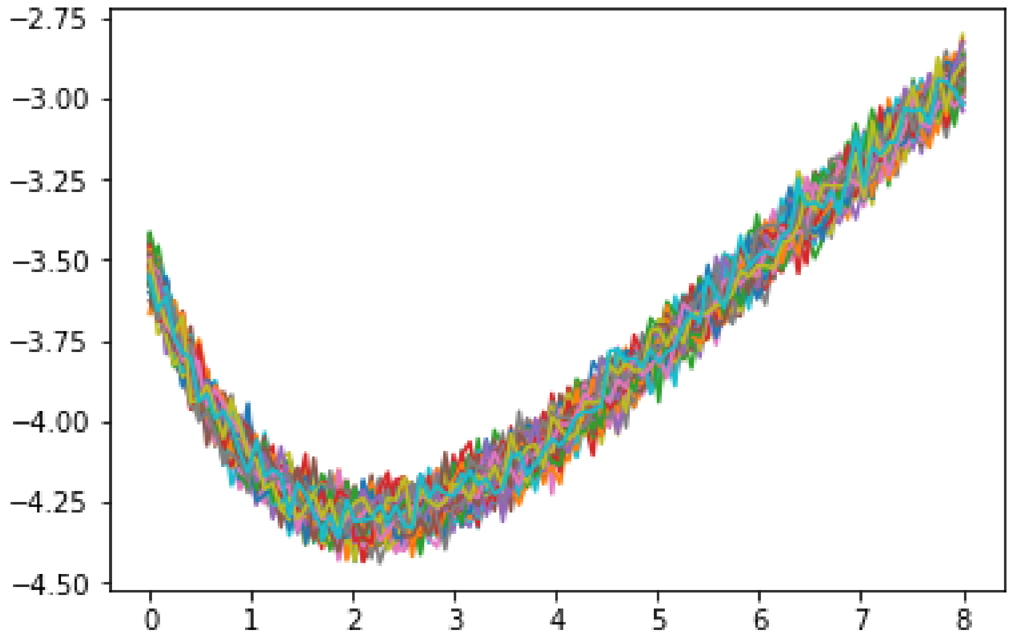

```
In [20]: hist(error, bins=20);
```



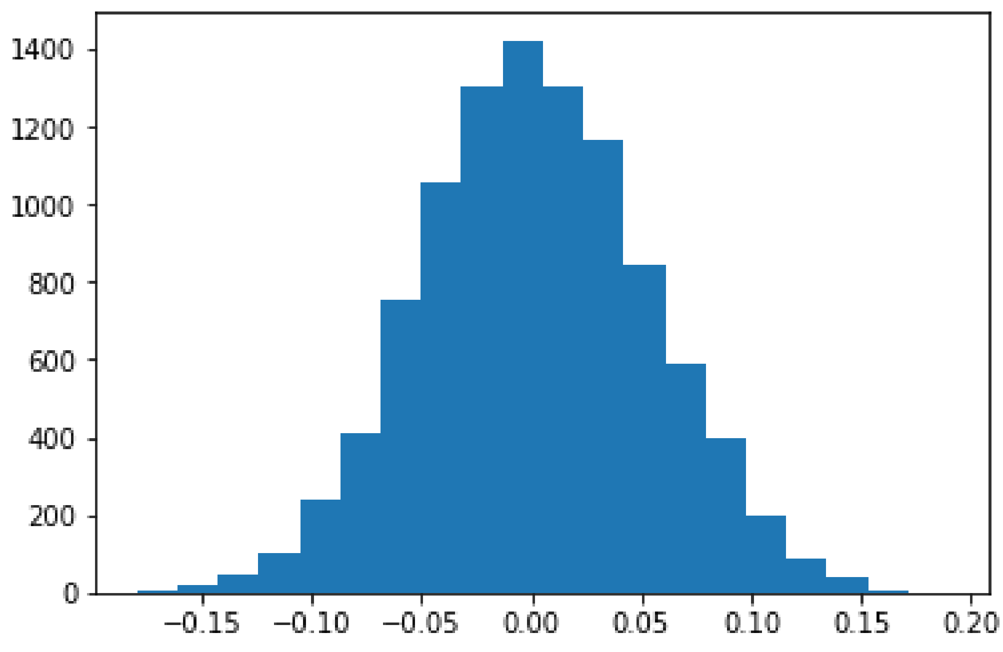

```
In [21]: def buildNoisySample():
             a = np.pi
             b = np.pi * 2.1
             nSamples = 100
             t = np.linspace(0, 8, nSamples)

             true_signal = modelFunction(a, b, t)
             noise = norm.rvs(loc=0, scale=0.05, size=nSamples)
             noisy_signal = true_signal + noise
             return t, noisy_signal
```

```
In [22]: allErrors = []
         for i in range(100):
             t, noisy_signal = buildNoisySample()
             plot(t, noisy_signal)
             error = noisy_signal - fitted_signal
             allErrors += error.tolist()
```




In [23]: hist(allErrors, bins=20);




```
In [24]: loc,scale = norm.fit(allErrors)
         print('Guessed noise characteristics: ')
```

```
print('Loc  : %.4f'%loc)
print('Scale: %.4f'%scale)
```

```
Guessed noise characteristics:
Loc  : 0.0016
Scale: 0.0518
```

## 5 Assignment -- tips

- Load the data corresponding to your group `./data/group_N.csv`, as we did with the sample
- Build your model function according to she simplified model:

$$M_z = M_0 \left| 1 - 2exp\left(-\frac{TI}{T1}\right) \right|$$

So there are two parameters to fit: $TI$ and $M_0$.