python Intermediate

Introduction to SciPy

Mauricio Sevilla

email= j.sevillam@uniandes.edu.co

22.04.19

Just as we saw how to interact with the `numpy` and `matplotlib` libreries on `python` , this week we will explore another one so called `SciPy` for Scientific Python.

As this course is thought to be for scientist, these tools are particularly relevant.

`SciPy` is one library with some routines implemented specially for science.

It is divided

Subpackage	Description
cluster	Clustering algorithms
constants	Physical and mathematical constants
fftpack	Fast Fourier Transforms routines
integrate	Integration and ODE solvers
interpolate	Interpolation and smoothing splines

Subpackage	Description
io	Input and Output
linag	Linear algebra
ndimage	N-dimensional image processing
ord	Orthogonal distance regression
optimize	Optimization and root-finding routines

Subpackage	Description
signal	Signal Processing
sparse	Sparse matrices and associated routines
spatial	Spatial data structures and algorithms
special	Special functions
stats	Statistical distributions and functions

We can explore some of them in order to understand how libraries on python are used and how to read the docs!. [SciPy Docs (https://docs.scipy.org/doc/)](https://docs.scipy.org/doc/)

During the course, everytime that we have used `numpy`, we have imported it with an alias, such as,

In [1]:
```python
import numpy as np
```

And it allows us to use every part of numpy by using `np.` in front of the instruction, for instance `np.pi` or `np.array()`

`scipy` is constructed from different sub-modules, so it is not usually imported the same way `numpy` is. It is usual to import the submodules

```python
from scipy import ASubModule
```

let us see a couple of examples, from the `special` submodule

One of the most widely used modules of `scipy` is the `scipy.special` because it allows us to use some special functions that are not *easy* to define by our own.

Special

http://scipy.github.io/devdocs/special.html (http://scipy.github.io/devdocs/special.html)

In [2]:

```
import numpy as np
import matplotlib.pylab as plt
from scipy import special
%config InlineBackend.figure_format = 'retina'
import matplotlib as mpl
mpl.rcParams['mathtext.fontset'] = 'cm'
```

Gamma function $\Gamma(z)$

Is a complex defined function, which correspond to the factorial for z a real integer

$$\Gamma(z) = \int_{\infty}^{\infty} t^{z-1} e^{-t} dt$$

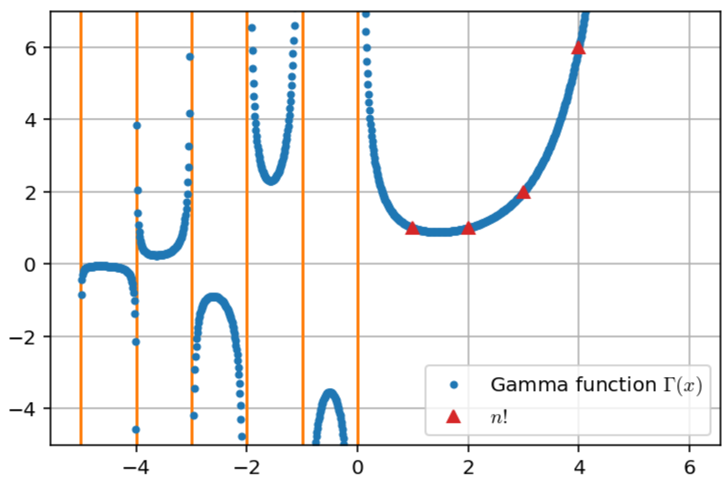
In [3]:

```
x=np.linspace(-5,5,1000)
y=special.gamma(x)
```

In [4]:
```
fig=plt.figure()
ax=fig.add_subplot(111)
ax.set_ylim(-5,7)
k = np.arange(1, 7)
for i in range(-5,1):
    ax.axvline(i,color='C1')
ax.plot(x,y,'.',label='Gamma function $\Gamma(x)$')

plt.plot(k, special.factorial(k-1),'^',color='C3',label='$n!$')
ax.grid()
plt.legend()
```

Out[4]: <matplotlib.legend.Legend at 0x206eb6c4940>



Airy Functions

Solution of

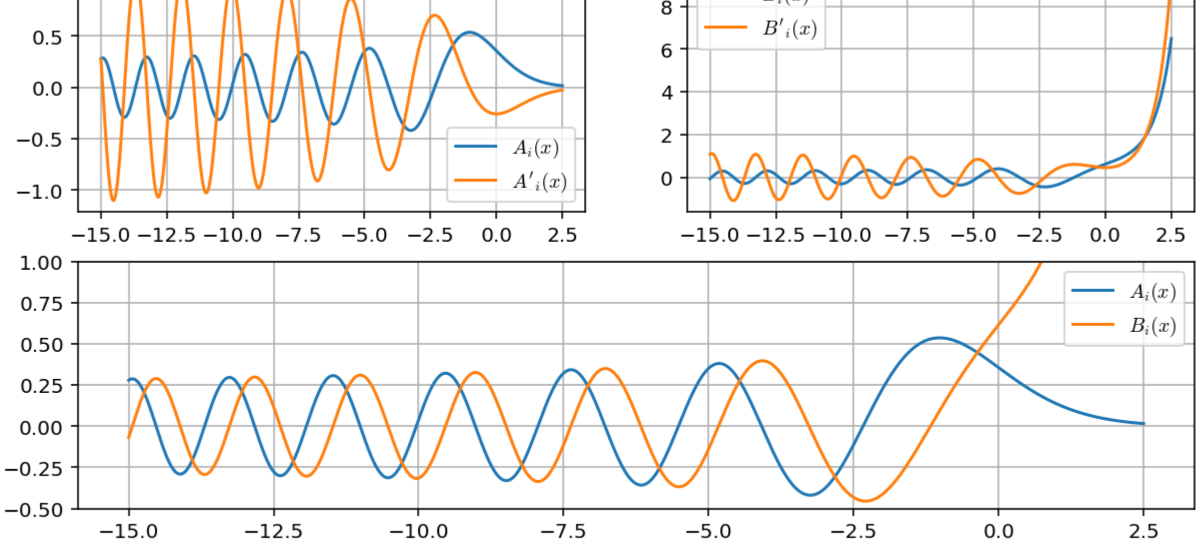
$$\frac{d^2y(x)}{dx^2} - xy = 0$$

In [5]:

```
x=np.linspace(-15,2.5,1000)
ai, aip, bi, bip=special.airy(x)
fig=plt.figure(figsize=(10,5))
ax1=fig.add_subplot(221)
ax1.plot(x,ai,label='$A_i(x)$')
ax1.plot(x,aip,label="$A'_i(x)$")
ax1.grid()
plt.legend()
ax2=fig.add_subplot(222)
ax2.plot(x,bi,label="$B_i(x)$")
ax2.plot(x,bip,label="$B'_i(x)$")
ax2.grid()
plt.legend()
ax3=fig.add_subplot(212)
ax3.set_ylim(-.5,1)
ax3.plot(x,ai,label="$A_i(x)$")
ax3.plot(x,bi,label="$B_i(x)$")
ax3.grid()
plt.legend()
```

Out[5]:

```
<matplotlib.legend.Legend at 0x206facbfc18>
```


$A_i(x)$
$A'_i(x)$
$B'_i(x)$
$A_i(x)$
$B_i(x)$

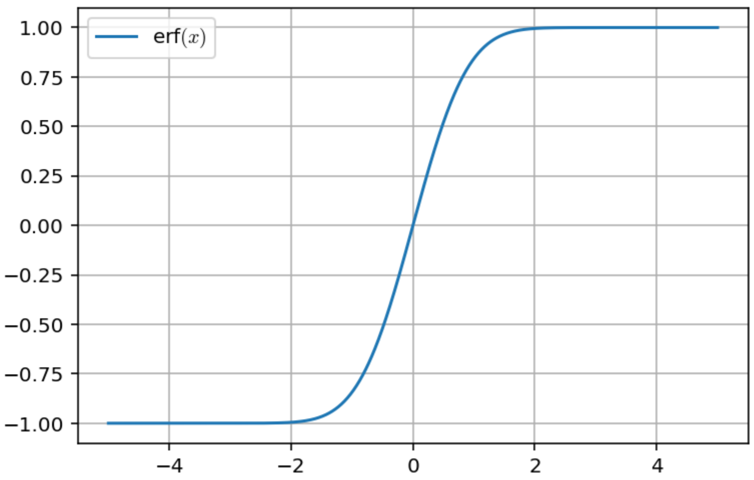
$\mathbf{erf}(x)$ Function

Very important in probability, due to it is the truncated integral of a gaussian.

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$$

In [6]:

```
x=np.linspace(-5,5,1000)
y=special.erf(x)
fig=plt.figure()
ax=fig.add_subplot(111)
ax.plot(x,y,label='erf$(x)$')
ax.grid()
plt.legend()
plt.show()
```



Special Polynomials

There are some polynimial families which were found while looking for solution for some EDO. Here we are going to see some of them WITHOUT talking about their properties.

Legendre Polynomials

Solution of the Legendre equation

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_n(x)}{dx}\right] + n(n+1)P_n(x) = 0$$

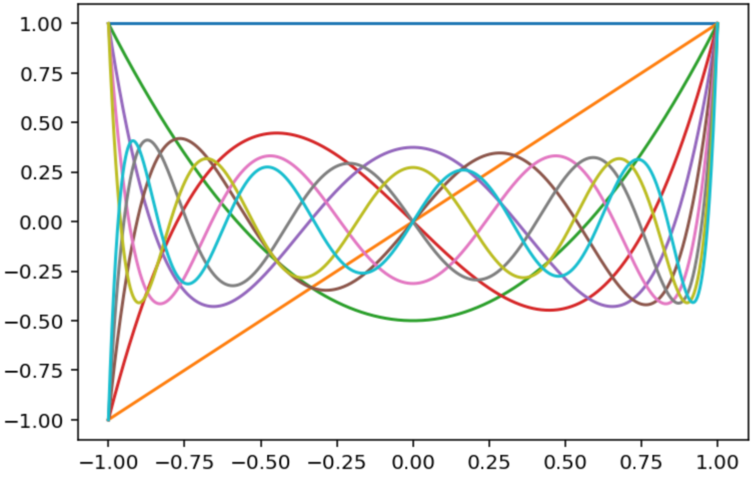
This equation becomes of interest when solving the **Laplace equation** on spherical coordinates.

$$\nabla^2 \varphi(\mathbf{r}) = 0$$

That means, all the electrostatic and magetostatic.

In [7]:

```
x=np.linspace(-1,1,1000)
for i in range(10):
    y=special.legendre(i)
    plt.plot(x,y(x))
plt.show()
```



Laguerre Polynomials

Solution of the Laguerre equation

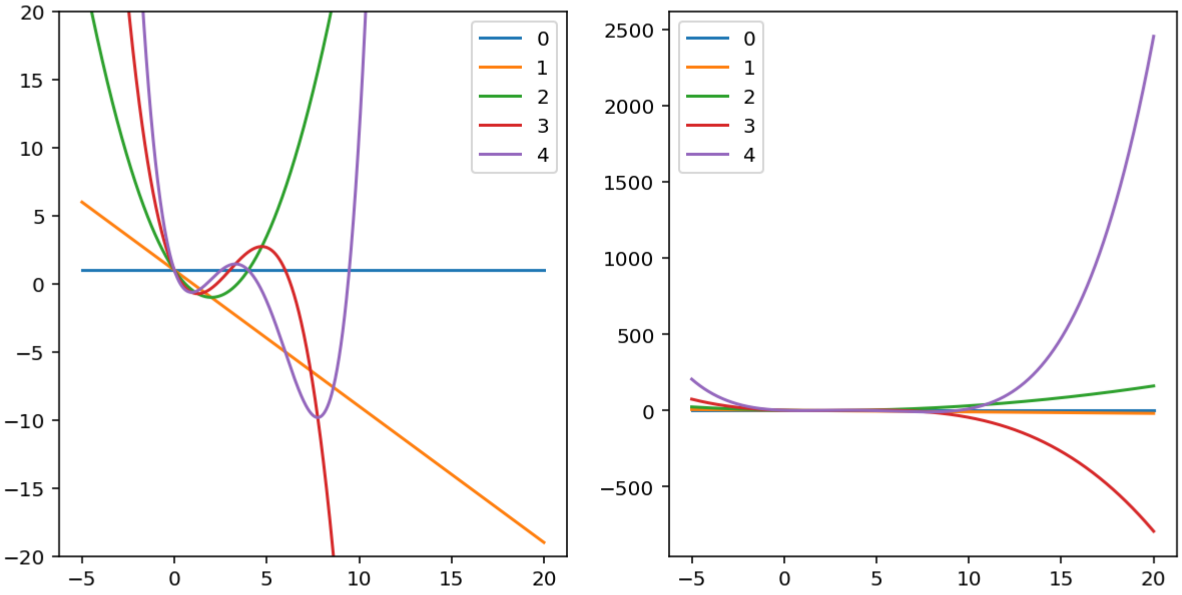
$$x\frac{d^2L_n(x)}{dx^2}+(1-x)\frac{dL_n(x)}{dx}+nL_n(x)=0$$

They arise in quantum mechanics on several problems,

- The radial equation of the Schrödinger equation for a single electron atom (Hydrogen).
- The static Wigner functions of oscillator systems in quantum mechanics in phase space.
- Solution for the Morse potential and of the 3D isotropic harmonic oscillator.

In [8]:

```
x=np.linspace(-5,20,1000)
fig=plt.figure(figsize=(10,5))
ax1=fig.add_subplot(121)
ax2=fig.add_subplot(122)
for i in range(5):
    y=special.laguerre(i)
    ax1.plot(x,y(x),label=str(i))
    ax1.set_ylim(-20,20)
    ax2.plot(x,y(x),label=str(i))
ax1.legend()
ax2.legend()
plt.show()
```



Hermite Polynomials

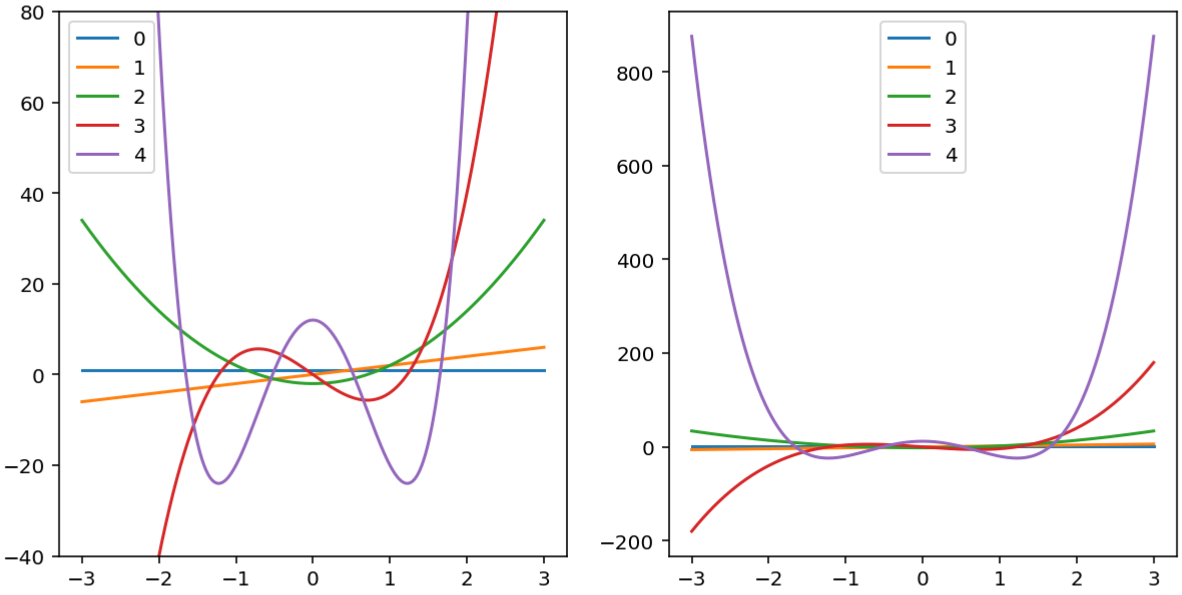
Solution of the Hermite equation

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$

Solution of the quantum harmonic oscillator.

In [9]:

```
x=np.linspace(-3,3,1000)
fig=plt.figure(figsize=(10,5))
ax1=fig.add_subplot(121)
ax2=fig.add_subplot(122)
for i in range(5):
    y=special.hermite(i)
    ax1.plot(x,y(x),label=str(i))
    ax1.set_ylim(-40,80)
    ax2.plot(x,y(x),label=str(i))
ax1.legend()
ax2.legend()
plt.show()
```



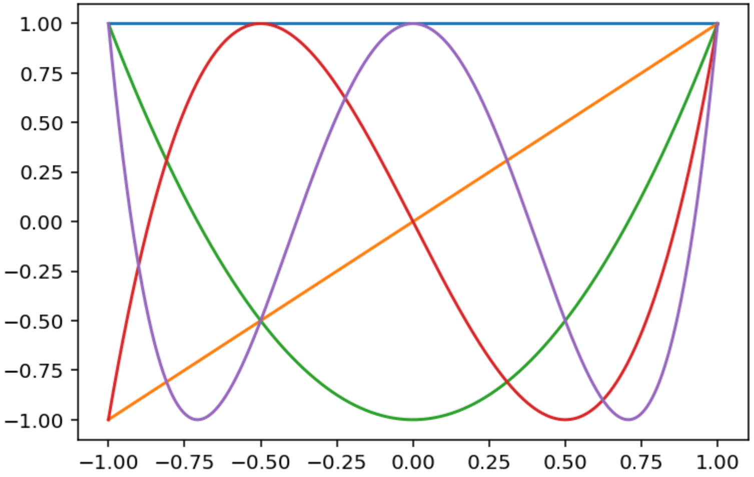
Chebyshev Polynomials (First Kind)

Are defined to be solution of

$$(1-x^2)\frac{d^2}{dx^2}T_n(x) - x\frac{d}{dx}T_n(x) + n^2 + T_n(x) = 0$$

In [10]:

```
x=np.linspace(-1,1,1000)
for i in range(5):
    y=special.chebyt(i)
    plt.plot(x,y(x))
plt.show()
```



Regression Analysis!!

One of the most important applications of programming on science is the data analysis.

This analysis may vary depending the area, but if we restrict ourselves to the experiments, the measurements used to test models and theories.

```
How can we know if our data follows a particular model?.
```

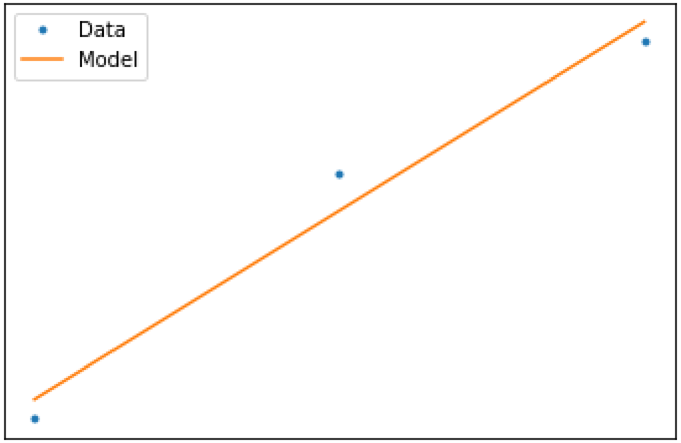
For example, we he have collected a set of data, and we want to know if it follows a straight line (That is our model), the question here splits into two parts

```
- Finding a unique line that describes the data given some criteria.
- Evaluating how good this line describes the data.
```

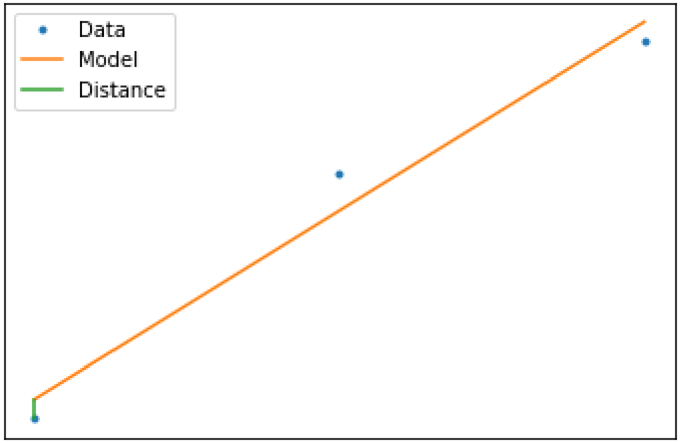
What can be a good criteria?

As we want to find a *unique* curve that describes the data, we must have some criteria so that the result choosen is the best according the criteria.

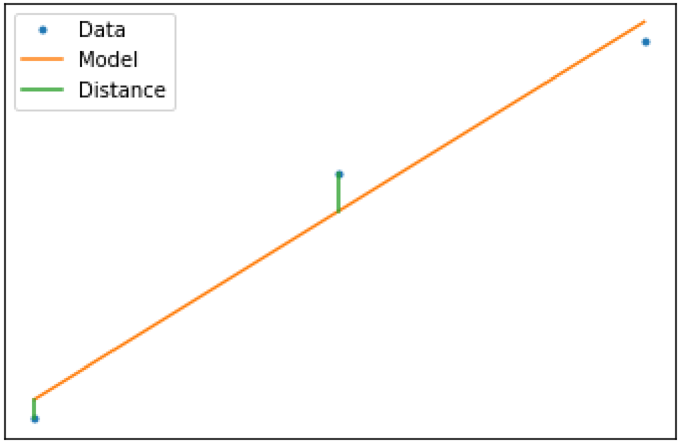
Least Squares Criteria



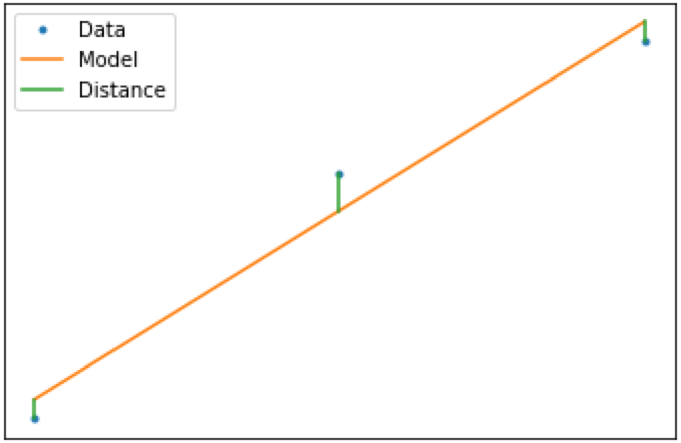
Least Squares Criteria



Least Squares Criteria



Least Squares Criteria



So the best line is the one that minimizes the vertical distance

$$\min_{\alpha}\left(\sum_{i}(f(x_i,\alpha)-y_i)^2\right)$$

When we have a linear model, this minimization can be calculated using a formula, such that

$$f(x) = ax + b$$

where the parameters can be calculated as,

$$a = \frac{\sum_i y_i \sum_i (x_i^2) - \sum_i x_i \sum_i (x_i y_i)}{N \sum_i (x_i^2) - (\sum_i x_i)^2}$$

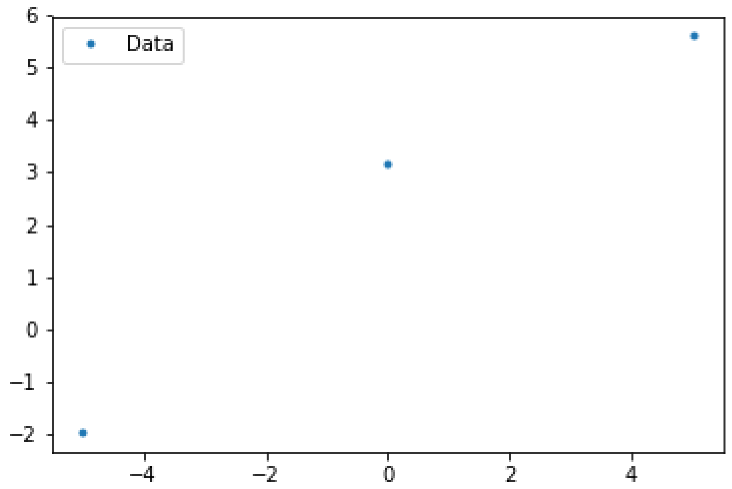
and

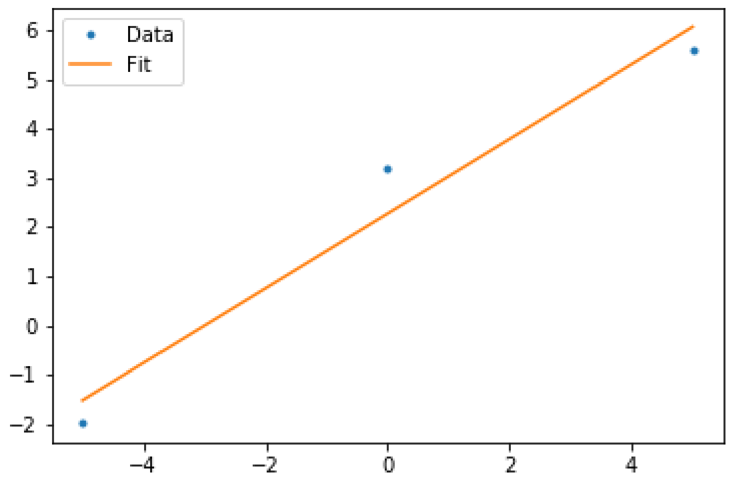
$$b = \frac{N \sum_i (x_i y_i) - \sum_i x_i \sum_i y_i}{N \sum_i (x_i^2) - (\sum_i x_i)^2}$$

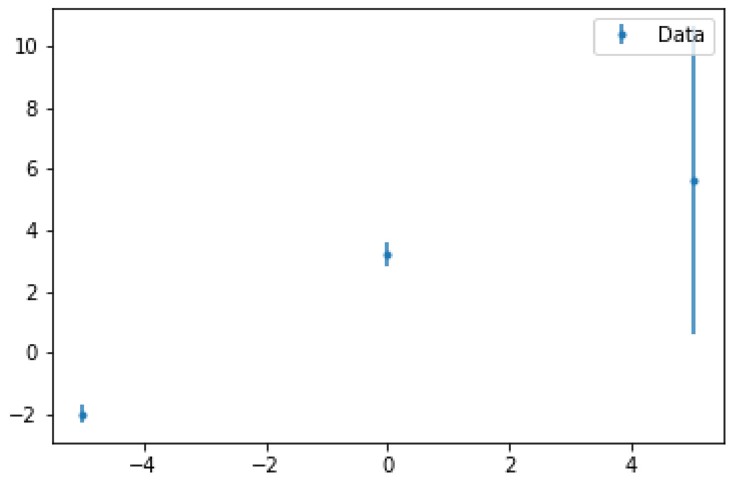
Experimental data

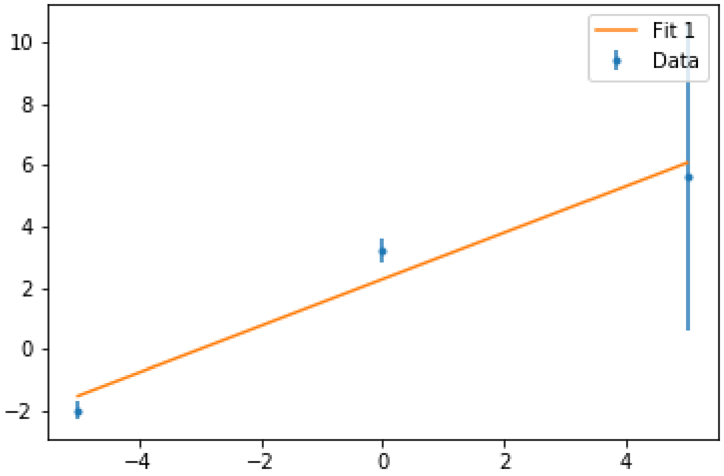
Have error bars!, that means that

- Data with small error weights more
- Data with big error weights less

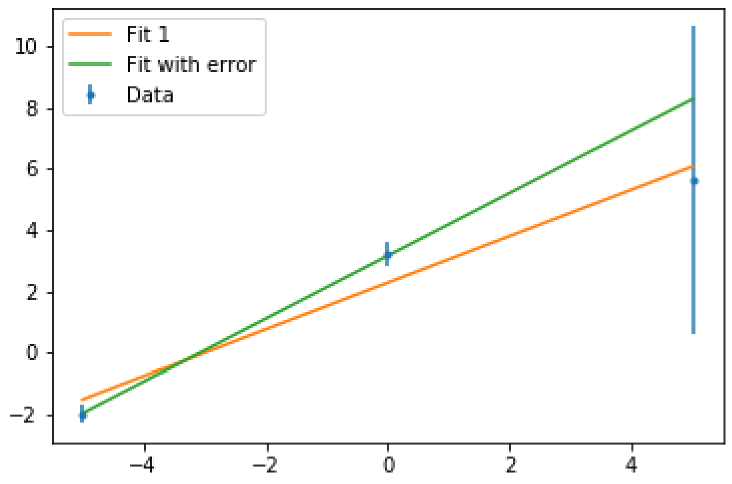

Data
6
5
4
3
2
1
0
−1
−2
−4
−2
0
2
4


Data
Fit
6
5
4
3
2
1
0
−1
−2
−4
−2
0
2
4


Data
10
8
6
4
2
0
−2
−4
−2
0
2
4



10
8
6
4
2
0
−2
−4
−2
0
2
4
Fit 1
Data



Fit 1
Fit with error
Data
10
8
6
4
2
0
−2
−4
−2
0
2
4

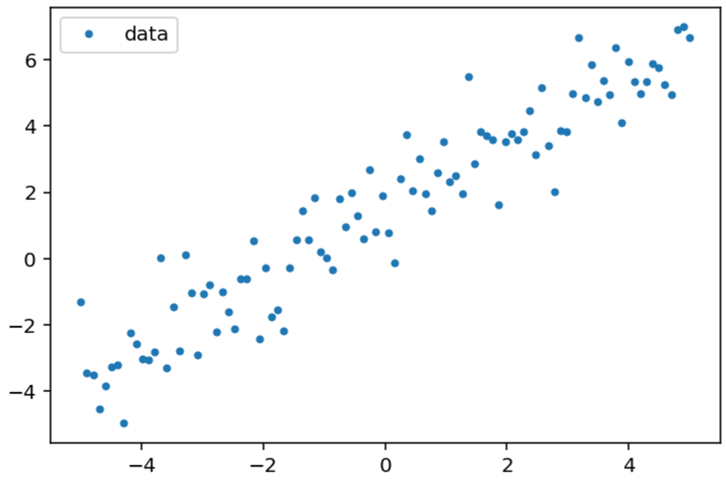
How can we use these ideas with `python` ?.

There are several ways, but we are going to concentrate on one very robust method of `SciPy` , curve_fit (http://scipy.github.io/devdocs/generated/scipy.optimize.curve_fit.html).

In [11]:

```
x,y,err=np.genfromtxt('https://raw.githubusercontent.com/jmsevillam/Herramientas-Computacionales-UniAndes/master/Data/data_fit.dat')
```

In [12]:
```
fig=plt.figure()
ax=fig.add_subplot(111)
ax.plot(x,y,'.',label='data')
plt.legend()
plt.show()
```



In [13]:

```
from scipy.optimize import curve_fit
```

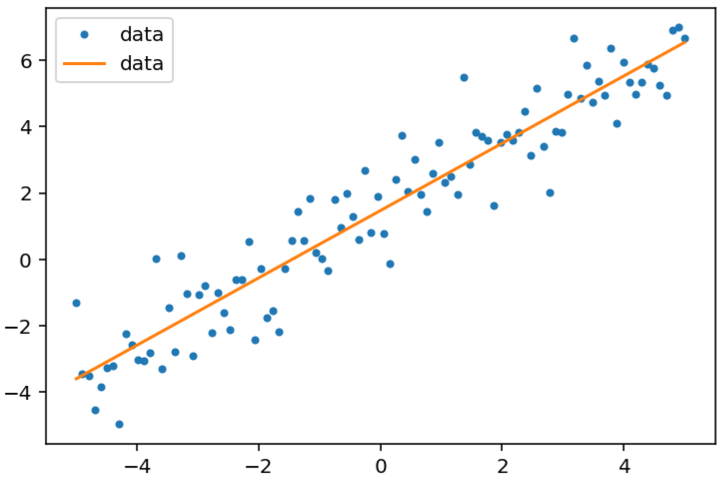
In [14]:

```
def fit(x,a,b):
    return a*x+b
```

In [15]:

```
popt,pcov=curve_fit(fit,x,y)
```

In [16]:
```
fig=plt.figure()
ax=fig.add_subplot(111)
ax.plot(x,y,'.',label='data')
ax.plot(x,fit(x,*popt),'-',label='data')
plt.legend()
plt.show()
```



In [17]:
```
print(popt,pcov.diagonal()**0.5)
```

```
[1.01417833 1.47199575] [0.03395194 0.09899587]
```

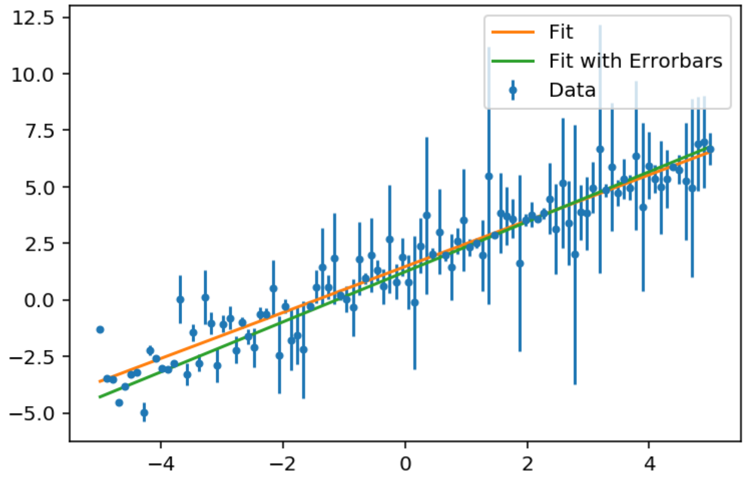
In [18]:

```
popt2,pcov2=curve_fit(fit,x,y,sigma=err)
print(popt2,pcov2.diagonal()**0.5)
```

```
[1.10593441 1.24217778] [0.02733564 0.12563067]
```

In [19]:

```
fig=plt.figure()
ax=fig.add_subplot(111)
ax.errorbar(x,y,err,fmt='.',label='Data')
ax.plot(x,fit(x,*popt),'-',label='Fit')
ax.plot(x,fit(x,*popt2),'-',label='Fit with Errorbars')
plt.legend()
plt.show()
```



In [20]:
```
print(popt,pcov.diagonal()**0.5,popt2,pcov2.diagonal()**0.5)
```

```
[1.01417833 1.47199575] [0.03395194 0.09899587] [1.10593441 1.24217778] [0.02733564
0.12563067]
```