Scipy

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Scipy

- Scipy (Scientific Python), provides numerous scientific and engineering utilities needed for mathematical operations (e.g. Bessel functions, optimization routines etc.)
- In this respect, Scipy is similar to the toolboxes in Matlab and consists of functions that form the scipy module.
- Scipy module is organized in sub modules and those submodules need to be imported before use.
- Similar to Numpy, Scipy is not a built-in modeule and need to be installed separately and imported before use.
- Many of Scipy functions (if not all) depend on the Numpy arrays both for input/output.

Scipy

Some of the Scipy sub modules:

scipy.cluster	Cluster Analysis
scipy.constants	Matematical and physical constants
scipy.fftpack	Fast Fourier Transformation
scipy.integrate	Integration routines
scipy.interpolate	Interpolation
scipy.io	IO
scipy.linalg	Linear Algebra Utilities
scipy.ndimage	n-dimensional image module
scipy.odr	Orthogonal Distance Regression
scipy.optimize	Optimization
scipy.signal	Signal Processing
scipy.sparse	Sparse Matrices
scipy.spatial	Spatial Data Structures and Algorithms
scipy.special	Special Matrix Functions
scipy.stats	Statistical Functions

Scipy.io

- Scipy heavily depends on Numpy data structures.
- Scipy.io provides several useful practical I/O functions
- For instance Matlab *.mat files can be read and written directly in Python:

Scipy.io

Similarly, various image formats can be read directly:

```
from scipy import misc misc.imread('fname.png') array(...)
```

Remember Numpy also has file reading utilities:

```
numpy.loadtxt()/numpy.savetxt()
numpy.genfromtxt()/numpy.recfromcsv()
```

Numpy has its own binary format (similar to Matlab mat files) and its compressed form for fast reading/saving and disk size efficiency

```
numpy.save()/numpy.load()
numpy.savez() → for saving in binary 'npz' files
```

- Scipy.linalg is based on highly optimized linear algebra libraries ATLAS LAPACK and BLAS.
- Numpy also has a linear algebra library.
- However, Scipy is not only more comprehensive but also more optimized and efficient for large scale problems.
- Since Scipy Linear Algebra modüle is based on LAPACK and BLAS, it is also much faster than Numpy.linalg modüle.
- Use Scipy Lineary Algebra whenever possible.

- Scipy.linalg provides a comprehensive set of linear algebra functions.
- Example usage:

```
from scipy import linalg
arr = np.array([[1, 2], [3, 4]])
linalg.det(arr)
-2.0
iarr = linalg.inv(arr)
iarr
array([[-2., 1.],
       [1.5, -0.5]
```

Scipy.linalg.det

$$|\mathbf{A}| = \sum_{j} (-1)^{i+j} a_{ij} M_{ij}.$$
 $\mathbf{A} = \begin{bmatrix} 1 & 3 & 5 \ 2 & 5 & 1 \ 2 & 3 & 8 \end{bmatrix}$
 $|\mathbf{A}| = 1 \begin{vmatrix} 5 & 1 \ 3 & 8 \end{vmatrix} - 3 \begin{vmatrix} 2 & 1 \ 2 & 8 \end{vmatrix} + 5 \begin{vmatrix} 2 \ 2 & 3 \end{vmatrix}$
 $= 1 (5 \cdot 8 - 3 \cdot 1) - 3 (2 \cdot 8 - 2 \cdot 1) + 5 (2 \cdot 3 - 2 \cdot 5) = -25.$

import numpy as np
from scipy import linalg
arr = np.array([[1, 3,5],[2,5,1],[2,3,8]])
linalg.det(arr)
-25.0

Scipy.linalg.inv

$$\mathbf{A} = \begin{bmatrix} 1 & 3 & 5 \\ 2 & 5 & 1 \\ 2 & 3 & 8 \end{bmatrix} \qquad \mathbf{A}^{-1} = \frac{1}{25} \begin{bmatrix} -37 & 9 & 22 \\ 14 & 2 & -9 \\ 4 & -3 & 1 \end{bmatrix} = \begin{bmatrix} -1.48 & 0.36 & 0.88 \\ 0.56 & 0.08 & -0.36 \\ 0.16 & -0.12 & 0.04 \end{bmatrix}$$

Many complex linear algebra routines (e.g. Singular Value Decompositon etc.) are also available:

```
arr = np.arange(9).reshape((3, 3)) + np.diag([1, 0, 1]) uarr, spec, vharr = linalg.svd(arr)
```

- While only SVD, QR and Eigen Decomposition is presented here, there are many others available including:
 - **LU**
 - Cholesky
 - Schur matrix factorization

Let's solve the linear equation above with scipy.linalg:

```
import numpy as np
from scipy import linalg
A = np.array([[1, 3,5],[2,5,1],[2,3,8]])
b = np.array([[10], [8],[3]])
linalg.inv(A).dot(b) OR linalg.inv(A) @ b
array([[-9.28], [5.16],[ 0.76]])
```

▶ A faster solution can be achieved by using "solve":

```
import numpy as np
from scipy import linalg
A = np.array([[1, 3,5],[2,5,1],[2,3,8]])
b = np.array([[10], [8],[3]])
np.linalg.solve(A, b)
array([[-9.28], [5.16],[ 0.76]])
```

Scipy.linalg Matrix/Vector Norms

$$\|\mathbf{x}\| = \left\{egin{array}{ll} \max_{|x_i|} & \operatorname{ord} = \inf \\ \min_{|x_i|} & \operatorname{ord} = -\inf \\ \left(\sum_i |x_i|^{\operatorname{ord}}
ight)^{1/\operatorname{ord}} & |\operatorname{ord}| < \infty \cdot \|\mathbf{A}\| = \left\{egin{array}{ll} \max_i \sum_j |a_{ij}| & \operatorname{ord} = -\inf \\ \max_j \sum_i |a_{ij}| & \operatorname{ord} = 1 \\ \min_j \sum_i |a_{ij}| & \operatorname{ord} = -1 \\ \max \sigma_i & \operatorname{ord} = 2 \\ \min \sigma_i & \operatorname{ord} = -2 \\ \sqrt{\operatorname{trace}\left(\mathbf{A}^H \mathbf{A}
ight)} & \operatorname{ord} = \operatorname{'fro'} \end{array}
ight.$$

import numpy as np from scipy import linalg A=np.array([[1,2],[3,4]])

linalg.norm(A) \rightarrow 5.4772255750516612

linalg.norm(A,'fro') \rightarrow 5.4772255750516612

linalg.norm(A,1) \rightarrow 6

linalg.norm(A,-1) \rightarrow 4

linalg.norm(A,np.inf) \rightarrow 7

Scipy.linalg Least Squares Solution

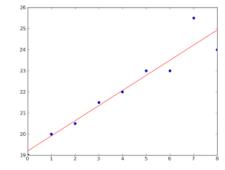
$$\|(w_1x_i+w_2)-y_i\|^2 egin{pmatrix} x_1 & 1 \ x_2 & 1 \ \vdots & 1 \ \vdots & 1 \ x_n & 1 \end{pmatrix} \mathbf{w} = egin{pmatrix} y_1 \ y_2 \ \vdots \ \vdots \ \vdots \ y_n \end{pmatrix}$$

from numpy import arange, array, ones, linalg

$$xi = arange(0,9)$$

A = array([xi, ones(9)])

y = [19, 20, 20.5, 21.5, 22, 23, 23, 25.5, 24]



w = linalg.lstsq(A.T,y)[0] → doğrunun parametreleri ## w, resid, rank, sigma = linalg.lstsq(....)

Scipy.linalg Generalized Matrix Inversion

- Generalized inverse of a matrix can be obtained through Moore-Penrose inverse function included in the Scipy.linalg module.
- Two different algorithms are available for Moore-Penrose inverse:
 - pinv (based on least-squares)
 - pinv2 (based on SVD)

```
A = floor(random.rand(4,4)*20-10)
b = floor(random.rand(4,1)*20-10) \rightarrow Ax=b
pinv = linalg.pinv(A)
xPinv = dot(pinv,b)
```

Scipy.linalg Singular Value Decomposition (SVD)

- Singular Value Decomposition is one of the most powerful algorithms in Linear Algebra.
- SVD can be used to analyze vector spaces or illconditioned problems.
- One particular application is the Moore-Penrose inverse.
- The problem in the previous slide can solved explicitly by SVD as follows:

```
A = floor(random.rand(4,4)*20-10)
b = floor(random.rand(4,1)*20-10) → Ax=b
U,s,V = linalg.svd(A) # A'nın SVD Ayrıştırılması
pinv_svd = dot(dot(V.T,linalg.inv(diag(s))),U.T)
```

Scipy.linalg QR Factorization

- QR Matrix Decomposition (Factorization) is also another powerful method for linear equations.
- The equation in the previous slide can also be solved through QR as follows:

$$||Ax - b||_2$$
 $QRx = b$ $Q^TQRx = Q^Tb$ $Rx = Q^Tb$

A = random.rand(5,3)

b = random.rand(5,1)

Q,R = linalg.qr(A)

Qb = dot(Q.T,b)

x qr = linalg.solve(R,Qb)

Scipy.linalg Eigenvalue/Eigenvector

 Eigenvalue Decomposition is also another popular matrix factorization method.

```
>>> import numpy as np
>>> from scipy import linalg
>>> A = np.array([[1, 2], [3, 4]])
>>> la, v = linalg.eig(A)
>>> |1, |2 = |a
>>> print(l1, l2) # eigen values
(-0.372281323269+0j) (5.37228132327+0j)
>>> print v[:, 0] # first eigen vector
[-0.82456484 0.56576746]
```

Scipy.fftpack

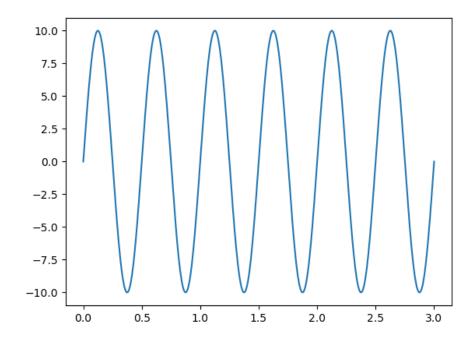
Scipy provides a very efficient Fast Fourier Transformation (FFT) modüle:

$$y[k] = \sum_{n=0}^{N-1} e^{-2\pi j rac{kn}{N}} x[n] \hspace{0.5cm} x[n] = rac{1}{N} \sum_{n=0}^{N-1} e^{2\pi j rac{kn}{N}} y[k]$$

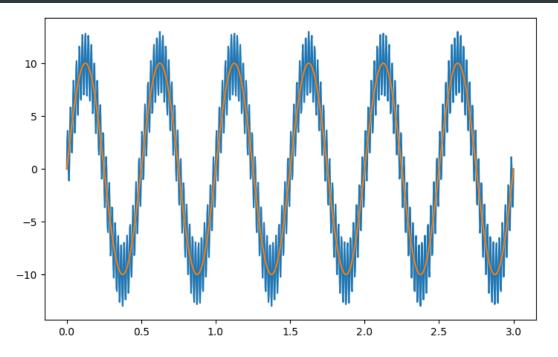
Scipy.fftpack

Scipy.fftpack containes other Fast Fourier related functions as well:

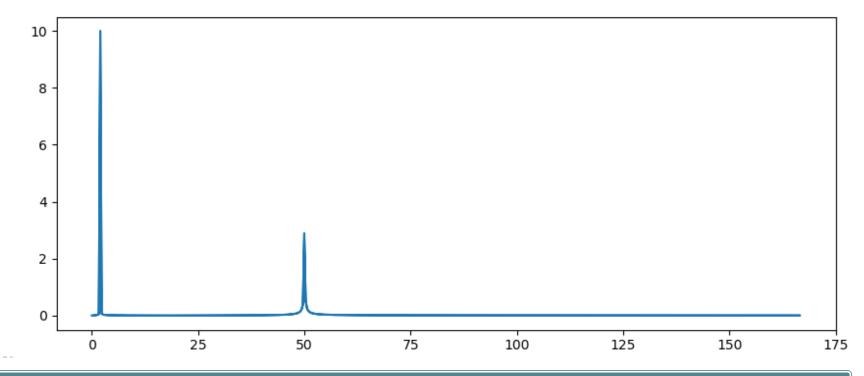
```
import numpy as np
time = np.linspace(0,3,1000,endpoint=True)
signal_freq = 2 # Signal Frequency
signal_amplitude = 10 # Signal Amplitude
signal = signal_amplitude*np.sin(2*np.pi*signal_freq*time)
```



```
noise_freq = 50 # Noise Frequency
noise_amplitude = 3 # Noise Amplitude
#Sine wave Noise
noise = noise_amplitude*np.sin(2*np.pi*noise_freq*time)
# Generated Signal with Noise
signal_noise = signal + noise
```

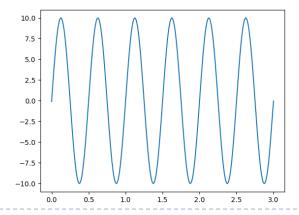


```
sig_noise_fft = fftpack.fft(signal_noise)
sig_noise_amp = 2 / time.size * np.abs(sig_noise_fft)
sig_noise_freq = np.abs(fftpack.fftfreq(time.size, 3/1000))
```



```
from scipy.signal import butter, filtfilt
# Filter requirements.
fs = 50.0  # sample rate, Hz
cutoff = 2  # Hz
order = 2  # sin wave can be approx represented as quadratic

def butter_lowpass_filter(data, cutoff, fs, order):
    print("Cutoff freq " + str(cutoff))
    nyq = 0.5 * fs # Nyquist Frequency
    normal_cutoff = cutoff / nyq
    # Get the filter coefficients
    b, a = butter(order, normal_cutoff, btype='low', analog=False)
    y = filtfilt(b, a,data)
    return y
# Filter the data, and plot filtered signals.
y = butter_lowpass_filter(signal_noise, 2, fs, order)
```



Scipy.optimize

Scipy.optimize provides local optimization algorithms (the most popular one is probably BFGS):

```
from scipy import optimize
def f(x):
  return x^**2 + 10*np.sin(x)
optimize.fmin bfgs(f, 0)
Optimization terminated successfully.
     Current function value: -7.945823
     Iterations: 5
     Function evaluations: 24
     Gradient evaluations: 8
array([-1.30644003])
```

Scipy.optimize

Scipy.optimize also provides several global optimization functions:

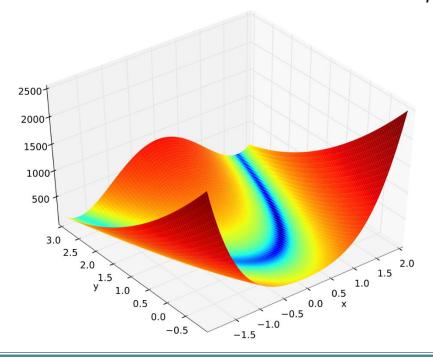
```
optimize.basinhopping(f, 0)
          nfev: 1725
minimization failures: 0
          fun: -7.9458233756152845
           x: array([-1.30644001])
        message: ['requested number of basinhopping
iterations completed successfully']
          njev: 575
          nit: 100
```

Unconstrained Optimization (minimize)

Rosenbrock function:

$$f(\mathbf{x}) = \sum_{i=1}^{N-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2.$$

The minimum of this function is obtained at $x_i=1$



Nelder-Mead Simplex algorithm (method='Nelder-Mead')

```
Optimization terminated successfully.

Current function value: 0.000000

Iterations: 339

Function evaluations: 571

[1. 1. 1. 1. ]
```

Powell Method (method='powell')

```
Optimization terminated successfully.

Current function value: 0.000000

Iterations: 18

Function evaluations: 1084

[1. 1. 1. 1. ]
```

Broyden-Fletcher-Goldfarb-Shanno algorithm (method='BFGS')

This method requires derivatives with respect to the parameters. The derivative is:

$$f(\mathbf{x}) = \sum_{i=1}^{N-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2.$$

$$egin{aligned} rac{\partial f}{\partial x_j} &= \sum_{i=1}^N 200 \left(x_i - x_{i-1}^2
ight) \left(\delta_{i,j} - 2 x_{i-1} \delta_{i-1,j}
ight) - 2 \left(1 - x_{i-1}
ight) \delta_{i-1,j}. \ &= 200 \left(x_j - x_{j-1}^2
ight) - 400 x_j \left(x_{j+1} - x_j^2
ight) - 2 \left(1 - x_j
ight). \end{aligned}$$

Broyden-Fletcher-Goldfarb-Shanno algorithm (method='BFGS')

```
import numpy as np
from scipy.optimize import minimize
def rosen(x):
    return sum(100.0*(x[1:]-x[:-1]**2.0)**2.0 + (1-x[:-1])**2.0)
def rosen der(x):
    xm = x[1:-1]
    xm m1 = x[:-2]
    xm p1 = x[2:]
    der = np.zeros like(x)
    der[1:-1] = 200*(xm-xm m1**2) - 400*(xm p1 - xm**2)*xm -
2*(1-xm)
    der[0] = -400*x[0]*(x[1]-x[0]**2) - 2*(1-x[0])
    der[-1] = 200*(x[-1]-x[-2]**2)
    return der
x0 = np.array([1.3, 0.7, 0.8, 1.9, 1.2])
res = minimize (rosen, x0, method='BFGS', jac=rosen der,
               options={'disp': True})
print(res.x)
```

```
Optimization terminated successfully.

Current function value: 0.000000

Iterations: 25

Function evaluations: 30

Gradient evaluations: 30

[1.00000004 1.0000001 1.00000021 1.00000044 1.00000092]
```

Newton-Conjugate-Gradient algorithm (method='Newton-CG')

This method requires second derivatives (Hessian) along with first derivates (Jacobian)

$$f\left(\mathbf{x}
ight)pprox f\left(\mathbf{x}_{0}
ight)+
abla f\left(\mathbf{x}_{0}
ight)\cdot\left(\mathbf{x}-\mathbf{x}_{0}
ight)+rac{1}{2}{\left(\mathbf{x}-\mathbf{x}_{0}
ight)}^{T}\mathbf{H}\left(\mathbf{x}_{0}
ight)\left(\mathbf{x}-\mathbf{x}_{0}
ight)$$

$$f(\mathbf{x}) = \sum_{i=1}^{N-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2.$$

$$egin{aligned} rac{\partial f}{\partial x_j} &= \sum_{i=1}^N 200 \left(x_i - x_{i-1}^2
ight) \left(\delta_{i,j} - 2 x_{i-1} \delta_{i-1,j}
ight) - 2 \left(1 - x_{i-1}
ight) \delta_{i-1,j}. \ &= 200 \left(x_j - x_{j-1}^2
ight) - 400 x_j \left(x_{j+1} - x_j^2
ight) - 2 \left(1 - x_j
ight). \end{aligned}$$

$$H_{ij} = rac{\partial^2 f}{\partial x_i \partial x_j} = 200 \left(\delta_{i,j} - 2 x_{i-1} \delta_{i-1,j}
ight) - 400 x_i \left(\delta_{i+1,j} - 2 x_i \delta_{i,j}
ight) - 400 \delta_{i,j} \left(x_{i+1} - x_i^2
ight) + 2 \delta_{i,j}, \ = \left(202 + 1200 x_i^2 - 400 x_{i+1}
ight) \delta_{i,j} - 400 x_i \delta_{i+1,j} - 400 x_{i-1} \delta_{i-1,j},$$

Newton-Conjugate-Gradient algorithm (method='Newton-CG')

```
from scipy.optimize import minimize
def rosen(x):
    return sum(100.0*(x[1:]-x[:-1]**2.0)**2.0 + (1-x[:-1])**2.0)
def rosen der(x):
    xm = x[1:-1]
    xm m1 = x[:-2]
    xm p1 = x[2:]
    der = np.zeros like(x)
    der[1:-1] = 200*(xm-xm m1**2) - 400*(xm p1 - xm**2)*xm - 2*(1-xm)
    der[0] = -400*x[0]*(x[1]-x[0]**2) - 2*(1-x[0])
    der[-1] = 200*(x[-1]-x[-2]**2)
    return der
def rosen hess(x):
    x = np.asarray(x)
    H = np.diag(-400*x[:-1],1) - np.diag(400*x[:-1],-1)
    diagonal = np.zeros like(x)
    diagonal[0] = 1200*x[0]**2-400*x[1]+2
    diagonal[-1] = 200
    diagonal[1:-1] = 202 + 1200*x[1:-1]**2 - 400*x[2:]
    H = H + np.diag(diagonal)
    return H
x0 = np.array([1.3, 0.7, 0.8, 1.9, 1.2])
                                                        Optimization terminated successfully.
res = minimize(rosen, x0, method='Newton-CG',
                                                               Current function value: 0.000000
               jac=rosen der, hess=rosen hess,
                                                               Iterations: 24
               options={ | xtol': 1e-8, 'disp': True})
                                                               Function evaluations: 33
                                                               Gradient evaluations: 33
print(res.x)
                                                               Hessian evaluations: 24
```

Constraints

Interval Constraints (bounds)

$$0 \le x_0 \le 1$$
 and $-0.5 \le x_1 \le 2.0$
from scipy.optimize import Bounds
bounds = Bounds([0, -0.5], [1.0, 2.0])

Linear Constraints

$$x_0+2x_1\leq 1$$
 and $2x_0+x_1=1$ $egin{bmatrix} -\infty\ 1\end{bmatrix}\leq egin{bmatrix} 1&2\ 2&1\end{bmatrix}egin{bmatrix} x_0\ x_1\end{bmatrix}\leq egin{bmatrix} 1\ 1\end{bmatrix}$

```
from scipy.optimize import LinearConstraint
linear_constraint = LinearConstraint([[1, 2], [2, 1]], [-np.inf, 1], [1, 1])
```

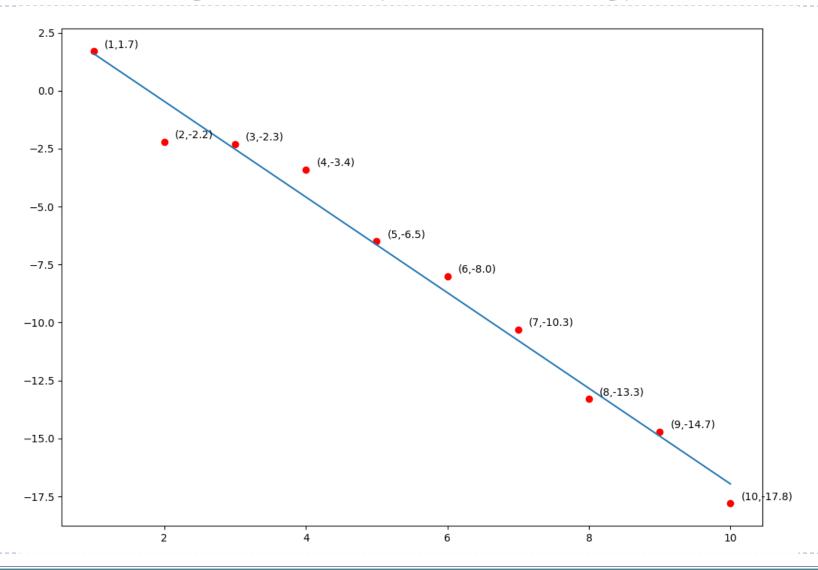
Trust-Region Constrained Algorithm

Interval-constrained solution algorithm is generally used for the problems as follows:

```
egin{array}{ll} \min_x & f(x) \ & 	ext{subject to:} & c^l \leq c(x) \leq c^u, \ & x^l \leq x \leq x^u. \end{array}
```

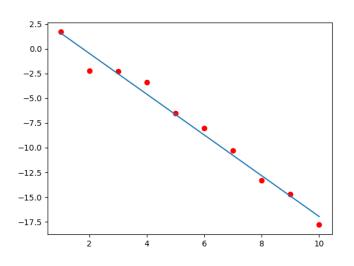
- Linear and non-linear constraints can be given together.
- First and second derivates can also be used.

Linear Regression (Line Fitting)



Linear Regression (Line Fitting)

```
import matplotlib.pyplot as plt
x = np.array([1,2,3,4,5,6,7,8,9,10])
y = np.array([1.7, -2.2, -2.3, -3.4, -6.5])
               -8.0, -10.3, -13.3,
               -14.7, -17.81)
A = []
for i in range(len(x)):
   A.append([1, x[i]])
A = np.array(A)
y = y.reshape(len(y),1)
a = np.linalq.pinv(A) @ y
ny = a[0][0] + a[1][0]*15
print(ny)
n1 = a[0][0] + a[1][0]*1
n2 = a[0][0] + a[1][0]*10
plt.plot([<mark>1,10</mark>],[n1,n2])
plt.scatter(x,y,color='red')
plt.show()
```

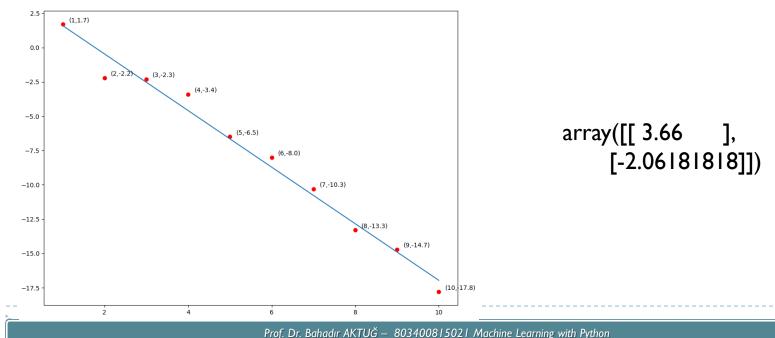


array([[3.66], [-2.06181818]])

-27.267272727273

▶ Let's solve the regression problem with Nelder-Mead method and Least-Squares.

```
x = np.array([1,2,3,4,5,6,7,8,9,10])
y = np.array([1.7,-2.2,-2.3,-3.4,-6.5,
-8.0,-10.3,-13.3,
-14.7,-17.8])
```



```
import numpy as np
                                                0.0
import matplotlib.pyplot as plt
from scipy.optimize import minimize
                                               -2.5
                                                              (4,-3.4)
                                                                  (5,-6.5)
x = np.array([1,2,3,4,5,6,7,8,9,10])
y = np.array([1.7, -2.2, -2.3, -3.4, -6.5,
                                                                         (7,-10.3)
                                               -10.0
           -8.0, -10.3, -13.3,
           -14.7, -17.81)
                                               -12.5
                                                                                  (9,-14.7)
                                               -15.0
def costFunc(coef):
                                               -17.5
    tot = 0
    for ix, iy in zip(x,y):
         tot += (coef[0] + coef[1] * ix - iy) * *2
    return tot
coef = np.array([1.0, 1.0])
res = minimize(costFunc, coef, method='nelder-mead',
                 options={ 'xatol': 1e-18, 'ftol':1E-18,
                 'maxfev':10000, 'disp': True})
print(res.x)
```

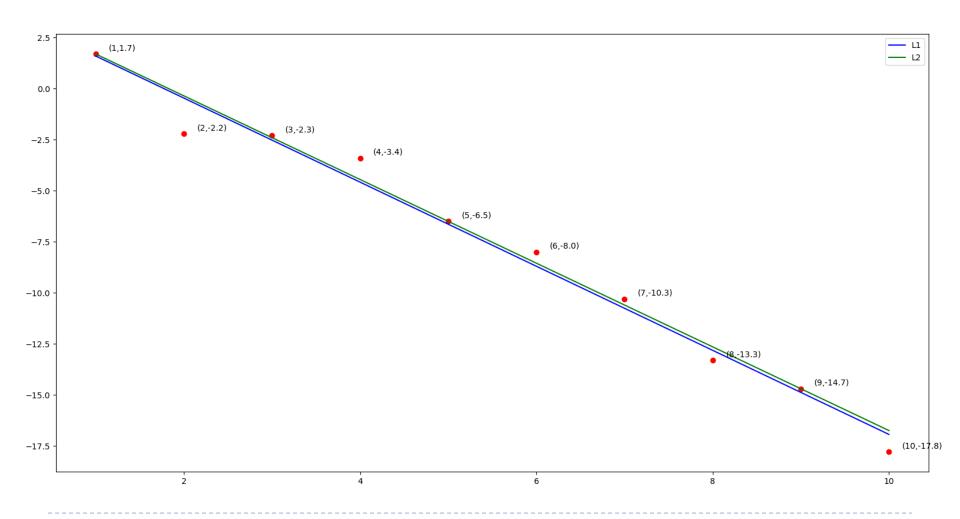
[3.65999998 -2.06181818]

Let's solve the regression problem with Nelder-Mead method but with L1 norm this time.

```
def costFunc(coef):
    tot = 0
    for ix,iy in zip(x,y):
        # tot += (coef[0]+coef[1]*ix - iy)**2
        tot += abs(coef[0]+coef[1]*ix - iy)
    return tot
```

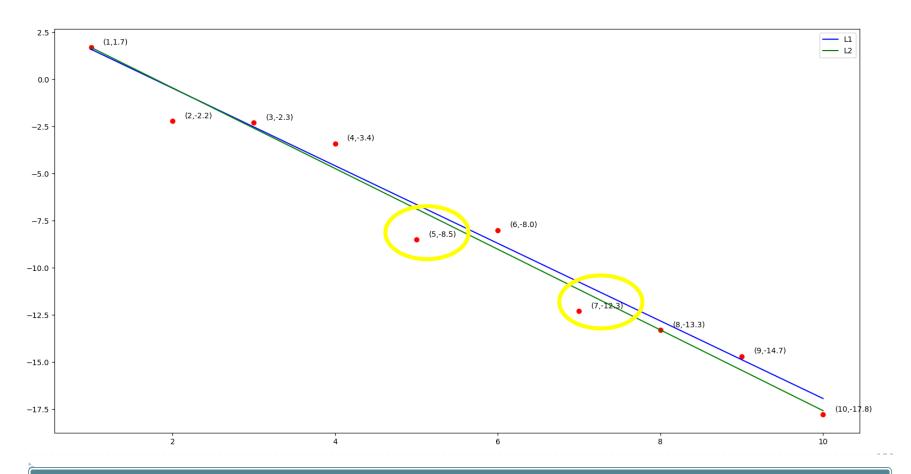
```
[3.75 - 2.05]
```

```
array([[ 3.66 ], [-2.06181818]])
```



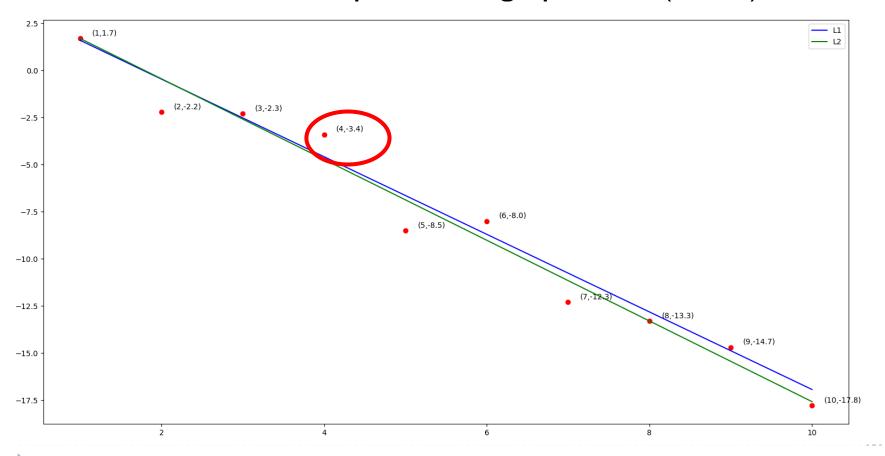
Doğrusal Regresyon (Nelder-Mead)

Değerleri değiştirerek çözelim.

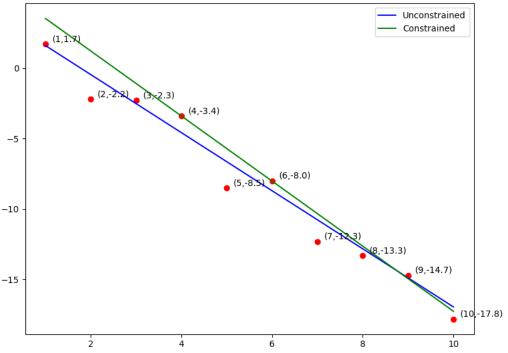


Linear Regression (Trust-Region Constrained Algorithm)

- Let's define a specific constraint.
- ▶ We want our line to pass through point at (4,-3.4).

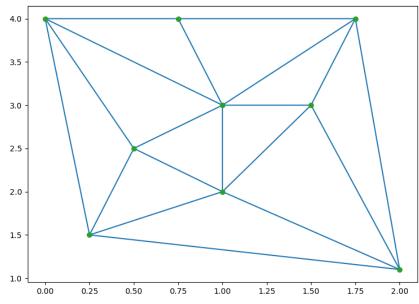


Linear Regression (Trust-Region Constrained Algorithm)



Number of iterations: 16, function evaluations: 36, CG iterations: 15, optimality: 1.56e-07, constraint violation: 4.44e -16, execution time: 0.032 s. [5.83047588 -2.30761897]

Scipy.spatial (Delaunay Triangulation)

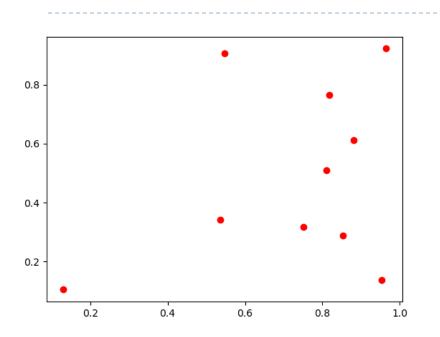


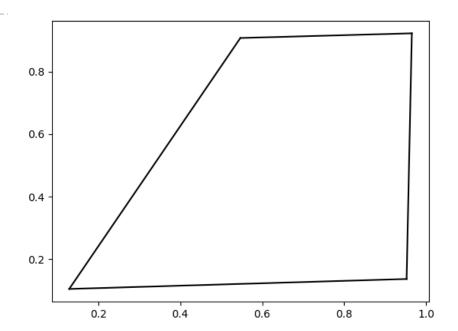
```
from scipy.spatial import Delaunay
import numpy as np
import matplotlib.pyplot as plt

points = np.array([[0,4],[2,1.1],[1,3],[1,2],[0.25,1.5],
   [0.75,4.0],[1.5,3.0],[1.75,4],[0.5,2.5]])

tri = Delaunay(points)
plt.triplot(points[:,0], points[:,1], tri.simplices.copy())
plt.plot(points[:,0], points[:,1], 'o')
plt.show()
```

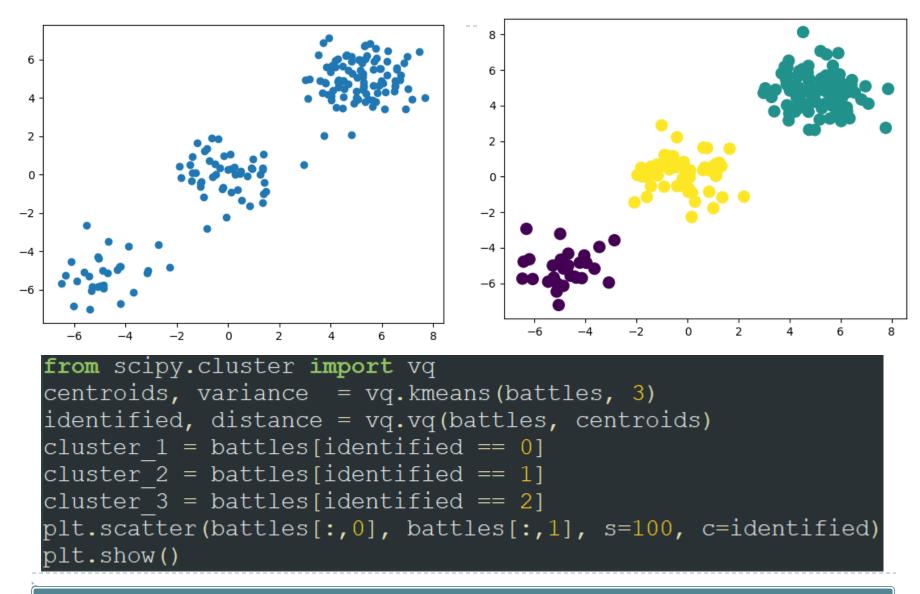
Scipy.spatial (Convex Hull)





```
from scipy.spatial import ConvexHull
import numpy as np
points = np.random.rand(10, 2) # 30 random points in 2-D
hull = ConvexHull(points)
import matplotlib.pyplot as plt
plt.plot(points[:,0], points[:,1], 'o')
for simplex in hull.simplices:
    plt.plot(points[simplex,0], points[simplex,1], 'k-')
plt.show()
```

Scipy.cluster (Spatial Grouping)



Scipy.interpolate

▶ For interpolation tasks, Scipy.interpolate can be used:

```
from scipy.interpolate import interp1d
measured_time = np.linspace(0, 1, 10)
noise = (np.random.random(10)*2 - 1) * 1e-1
measures = np.sin(2 * np.pi * measured_time) + noise
linear_interp = interp1d(measured_time, measures)
```

Scipy.interpolate

The interpolation can be implemented linearly, quadratically or cubicly:

```
from scipy.interpolate import interp1d
measured_time = np.linspace(0, 1, 10)
noise = (np.random.random(10)*2 - 1) * 1e-1
measures = np.sin(2 * np.pi * measured_time) + noise
cubic_interp = interp1d(measured_time, measures,
kind='cubic')
cubic_results = cubic_interp(computed_time)
```

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