# Lecture 21
# SciPy

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# Lecture 21 outline

Last time: NumPy

This time: SciPy

- overview of SciPy
- survey of SciPy modules

SciPy is an open source ecosystem that extends Python's functionality for math, science, and engineering

This ecosystem includes its open source software, its community, and its conferences

The SciPy library itself provides methods for signal processing, optimization, integration, statistics, and more

# SciPy library organization

| | | |
|---|---|---|
| → | cluster | Clustering algorithms |
| → | constants | Physical and mathematical constants |
| | fftpack | Fast Fourier Transform routines |
| → | integrate | Integration and ordinary differential equation solvers |
| | interpolate | Interpolation and smoothing splines |
| | io | Input and Output |
| | linalg | Linear algebra |
| | ndimage | N-dimensional image processing |
| | odr | Orthogonal distance regression |
| → | optimize | Optimization and root-finding routines |
| | signal | Signal processing |
| | sparse | Sparse matrices and associated routines |
| → | spatial | Spatial data structures and algorithms |
| | special | Special functions |
| → | stats | Statistical distributions and functions |

https://docs.scipy.org/doc/scipy/reference/tutorial/general.html

# *scipy.constants*

```
>>> from scipy import constants
>>> constants.pi                        # pi
3.141592653589793
>>> constants.golden                    # golden ratio, (1+5^.5)/2
1.618033988749895
>>> constants.Avogadro                  # Avogadro's number
6.022140857e+23
>>> constants.speed_of_light            # speed of light in vacuum
299792458.0
>>> constants.electron_mass             # mass of electron
9.10938356e-31
>>> constants.proton_mass               # mass of proton
1.672621898e-27
>>> constants.neutron_mass              # mass of neutron
1.674927471e-27
>>> scipy.constants.physical_constants  # returns dict of (values, units, precision)
{'Wien displacement law constant': (0.0028977685, 'm K', 5.1e-09),
 'atomic unit of 1st hyperpolarizablity': (3.20636151e-53, 'C^3 m^3 J^-2', 2.8e-60),
 'atomic unit of 2nd hyperpolarizablity': (6.2353808e-65, 'C^4 m^4 J^-3', 1.1e-71),
 'atomic unit of electric dipole moment': (8.47835309e-30, 'C m', 7.3e-37),
 'atomic unit of electric polarizablity': (1.648777274e-41, 'C^2 m^2 J^-1', 1.6e-49),
 'atomic unit of electric quadrupole moment': (4.48655124e-40, 'C m^2', 3.9e-47),
...
```

*Mathematical and (mostly) physical constants, units, and precisions*

https://docs.scipy.org/doc/scipy/reference/constants.html

## *scipy.stats*

Provides methods for numerous probability distributions and a wide variety of statistical operations

- probability distributions
- statistical tests
- frequency statistics
- summary statistics
- statistical distances
- contingency tables
- kernel density estimators

https://docs.scipy.org/doc/scipy/reference/stats.html

## distributions in *scipy.stats*

***Probability distributions*** assign relative frequencies to possible outcomes for random experiment – *e.g. a coin flip*

All *scipy.stats* distributions offer the same set of base functions:

- simulate random variates
- compute distribution probabilities for data
- compute moments (mean, variance, etc.)
- fit distribution parameters to data

https://docs.scipy.org/doc/scipy/reference/stats.html

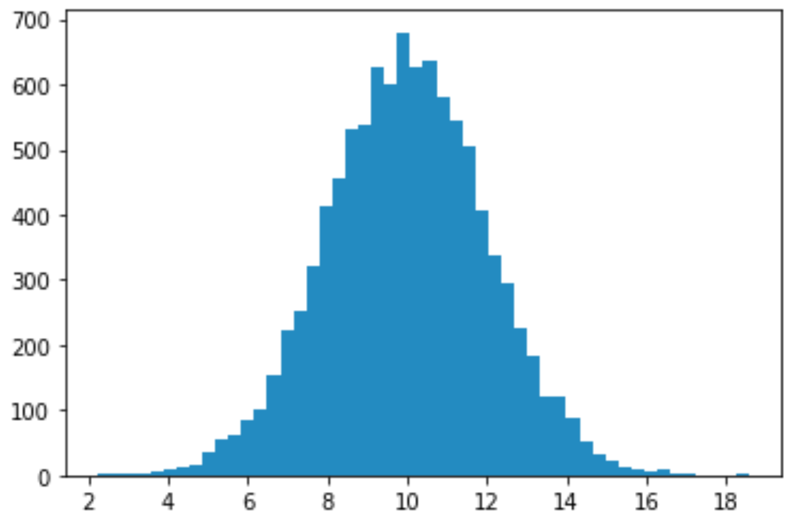
## distributions in *scipy.stats*

```
>>> from scipy import stats
>>> # distribution object
>>> stats.norm
<scipy.stats._continuous_distns.norm_gen object at 0x7fdf98b67d68>
>>> # generate 4 normal RVs
>>> x = stats.norm.rvs(loc=10,scale=2,size=4)
array([10.11179033, 10.10902411, 10.65111753, 10.32368948])
>>> stats.norm.pdf(x=x, loc=10, scale=2 )
array([0.19915978, 0.19917499, 0.18917553, 0.19687573])
>>> # return mean, variance, skewness, kurtosis (mvsk)
>>> stats.norm.stats(loc=10, scale=2, moments='mvsk')
(array(10.), array(4.), array(0.), array(0.))
>>> # generate 1000 normal RVs with mean=10, scale=2
>>> y = stats.norm.rvs(loc=10,scale=2,size=1000)
>>> # estimate mean and scale from simulated data
>>> stats.norm.fit( data=y, loc=50, scale=9
(9.939835173664239, 2.004585580838588)
```

https://docs.scipy.org/doc/scipy/reference/stats.html

# distributions in *scipy.stats*

```
>>> from scipy import stats
>>> import matplotlib
>>> import matplotlib.pyplot as plt
>>> # simulate 10000 RVs, mean=10, scale=2
>>> y = stats.norm.rvs(loc=10,scale=2,size=10000)
>>> y
array([13.23832222, 13.05731999, 7.30259037, ..., 9.8595785,
        9.46715211, 9.98579946])
>>> fig,ax = plt.subplots()
>>> p = ax.hist(y,bins=50)
>>> fig.show()
```



https://docs.scipy.org/doc/scipy/reference/stats.html

# distributions in *scipy.stats*

Roughly 100 distributions available,
each with different properties

| **Type** | **Name** | **Class** | **Use** |
|---|---|---|---|
| Continuous | uniform | *stats.uniform* | "flat" over interval |
| | normal | *stats.norm* | random sums |
| | exponential | *stats.expon* | events with rates |
| | beta | *stats.beta* | flexible on [0,1] |
| Discrete | bernoulli | *stats.bernoulli* | single coin-flip |
| | binomial | *stats.binom* | many coin-flips |
| | Poisson | *stats.poisson* | # events w/ rates |

https://docs.scipy.org/doc/scipy/reference/stats.html

# summary statistics in *scipy.stats*

Use ***summary statistics*** to describe simple properties of a data sample, *e.g. the sample mean*

```
>>> from scipy import stats
>>> import numpy as np
>>> x = stats.norm.rvs(loc=10, scale=2, size=1000)
>>> np.mean(x)                # sample mean
9.907750191507521
>>> stats.hmean(x)            # harmonic mean
9.4599529015089185
>>> stats.gmean(x)            # geometric mean
9.6924828402578722
>>> stats.sem(x)              # standard error of sample mean
0.06353084579162438
>>> stats.skew(x)             # sample skew (asymmetry)
0.011612124738411802
>>> stats.kurtosis(x)         # sample kurtosis (fat-tailedness)
-0.0055425614273967305
>>> stats.describe(x)         # give summary of sample data
DescribeResult(nobs=1000,
               minmax=(3.7313631618255805, 16.221776607589973),
               mean=9.907750191507521,
               variance=4.0361683669991582,
               skewness=0.011612124738411802,
               kurtosis=-0.0055425614273967305)
```

https://docs.scipy.org/doc/scipy/reference/stats.html

## statistical tests in *scipy.stats*

Many statistical tests that are used to analyze biological data are available, including:

- t-tests: *ttest_1samp, ttest_ind, ttest_rel*
- Chi-square*: chisquare*
- Kolmogorov-Smirnov: *kstest, ks_1samp, ks_2samp*
- Mann-Whitney: *mannwhitneyu*
- Cressie-Read power divergence: *power_divergence*
- Wilcox signed-rank test: *wilcoxon*
- Kruskal-Wallis H-test: *kruskal*

  *...and dozens more*

https://docs.scipy.org/doc/scipy/reference/stats.html

# Linear regression in *scipy.stats*

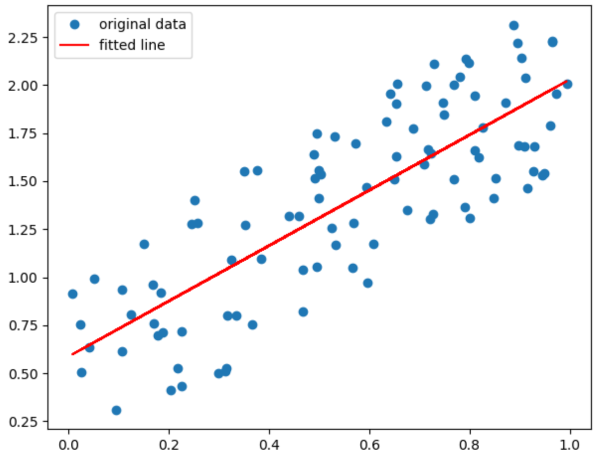
Fit data to line using slope and intercept parameters

```
>>> # import numpy and scipy
>>> import numpy as np
>>> import scipy as sp
>>> # simulate dataset
>>> np.random.seed(seed=12345)
>>> x = sp.stats.uniform.rvs(size=100, loc=0, scale=1)
>>> y = 1.6*x + sp.stats.uniform.rvs(size=100, loc=0, scale=1)
>>> # get results from linear regression, y ~ x
>>> res = sp.stats.linregress(x, y)
>>> res
LinregressResult(slope=1.4431933040436178, intercept=0.5860274273931283,
rvalue=0.8088733612574854, pvalue=2.4706574634065375e-24, stderr=0.1059730971193916,
intercept_stderr=0.06594536829897774)
>>> print(f"R-squared: {res.rvalue**2:.6f}")
R-squared: 0.65427
```

*regression*

```
>>> # plot results
>>> import matplotlib.pyplot as plt
>>> plt.plot(x, y, 'o', label='original data')
>>> plt.plot(x, res.intercept + res.slope*x, 'r',
label='fitted line')
>>> plt.legend()
>>> plt.show()
```

*plotting*



https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.linregress.html

# KDEs in *scipy.stats*

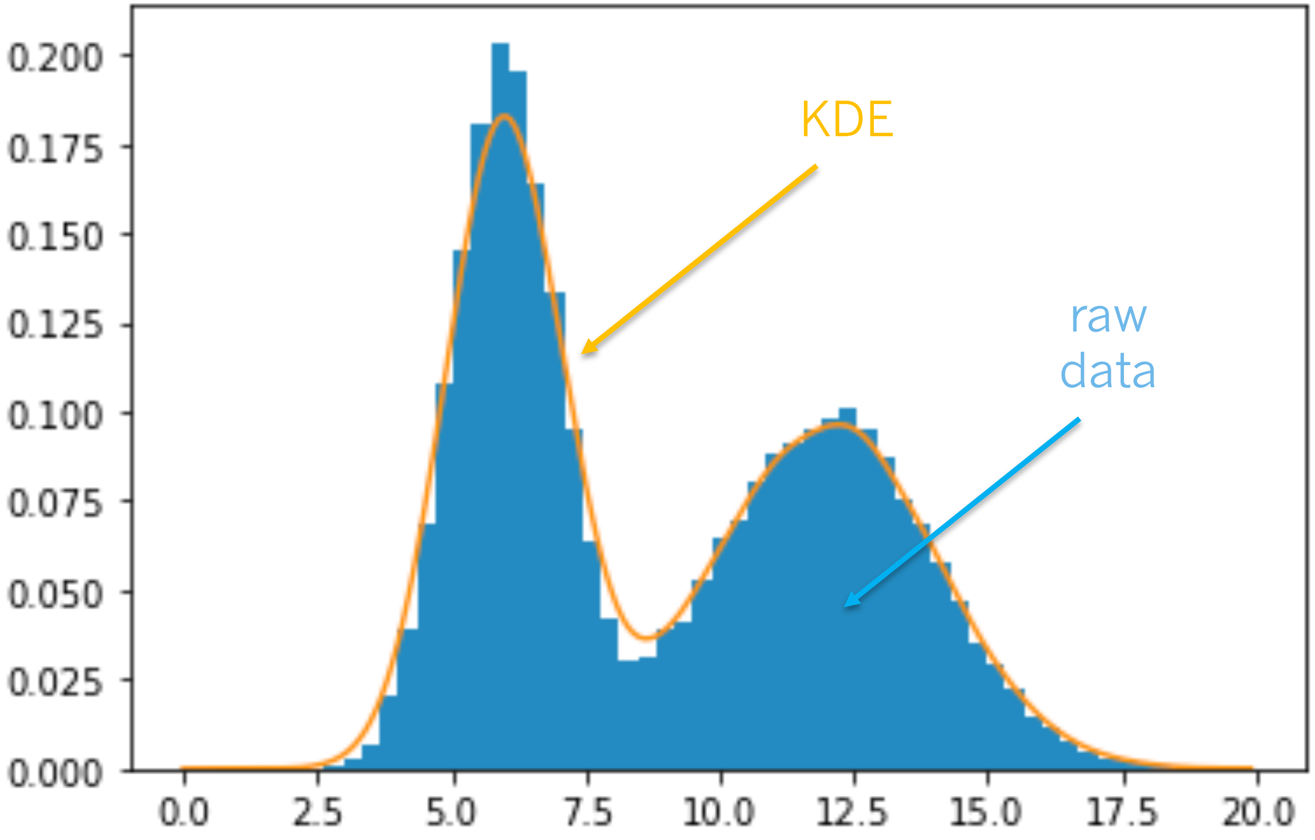
***Kernel density estimators*** (KDEs) approximate sample data as a continuous probability density

```
>>> from scipy import stats
>>> import matplotlib
>>> import matplotlib.pyplot as plt
>>> a = stats.norm.rvs(loc=12,scale=2,size=10000) # create samples, a
>>> b = stats.norm.rvs(loc=6,scale=1,size=10000)  # create samples, b
>>> z = np.append(a, b)       # mix samples a and b
>>> f = stats.gaussian_kde(z) # fit KDE object to data, z
>>> x = np.arange(0,20,0.1)   # range of input values for f()
>>> f(x)                      # density for each value, f(pos)
array([1.33471717e-11, 4.45526152e-11, 1.42288247e-10, 4.34870069e-10,
       1.27215449e-09, 3.56303164e-09, 9.55708453e-09, 2.45585700e-08,
       6.04813171e-08, 1.42815299e-07, 3.23510616e-07, 7.03432155e-07,
...
>>> fig,ax = plt.subplots()             # create empty plot
>>> h = ax.hist(z,bins=50,density=True) # plot histogram (normalized)
>>> ax.plot(x, f(x))                    # plot KDE curve
>>> plt.show()                          # show plot
```

https://docs.scipy.org/doc/scipy/reference/stats.html

# KDEs in *scipy.stats*

***Kernel density estimators*** (KDEs) approximate sample data as a continuous probability density

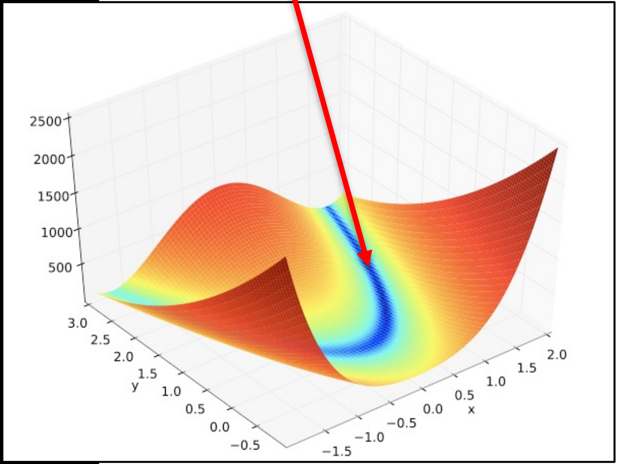


https://docs.scipy.org/doc/scipy/reference/stats.html

# *scipy.optimize*

```
>>> import numpy as np
>>> from scipy.optimize import minimize
>>> def rosen(x):
...   # Rosenbrock function, for a=1 and b=100
...   # f(x,y) = (1-x)^2 + 100*(y-x^2)^2
...   return (1.0-x[0])**2 + 100.0*(x[1]-x[0]**2.0)**2.0
>>>
>>> rosen( [1.0, 1.0] )        # optimal value, f(1,1)=0
0.0
>>> rosen( [1.01, 1.01] )      # worse value
0.010300999999999994
>>> rosen( [1.05, 1.05] )      # worse value
0.27812499999999999
>>> x0 = np.array([1.3, 0.7]) # initial guess
>>> # find the optimal value for x
>>> res = minimize(rosen, x0, method='nelder-mead',
                   options={'xatol': 1e-8, 'disp': True})
Optimization terminated successfully.
    Current function value: 0.000000
    Iterations: 79
    Function evaluations: 150
>>> print(res.x)               # estimate for x
[1. 1.]
>>> print(res.fun)             # minimum, approx 0.0
3.3736077629532093e-18
```

$$f(x,y) = (a-x)^2 + b(y-x^2)^2$$
$$a = 1, b = 100$$
$$f(1,1) = 0$$



https://docs.scipy.org/doc/scipy/reference/optimize.html

## *scipy.integrate*

Various methods to integrate functions,
fixed samples and ODEs

```
>>> from scipy import integrate
>>> # define function to integrate
>>> def x2(x):
...     return x**2
...
>>> # numerical integration using quadrature
>>> y, err = integrate.quad(x2, 0, 4)
>>> y
21.333333333333336     # numerical integrand
>>> err
2.368475785867001e-13  # numerical error
>>>
>>> print(4**3 / 3.)   # analytical result
21.3333333333
```

$$I = \int_0^4 x^2\,dx$$

$$= F(4) - F(0)$$

$$= \frac{4^3}{3} - \frac{0^3}{3} = 21\frac{1}{3}$$

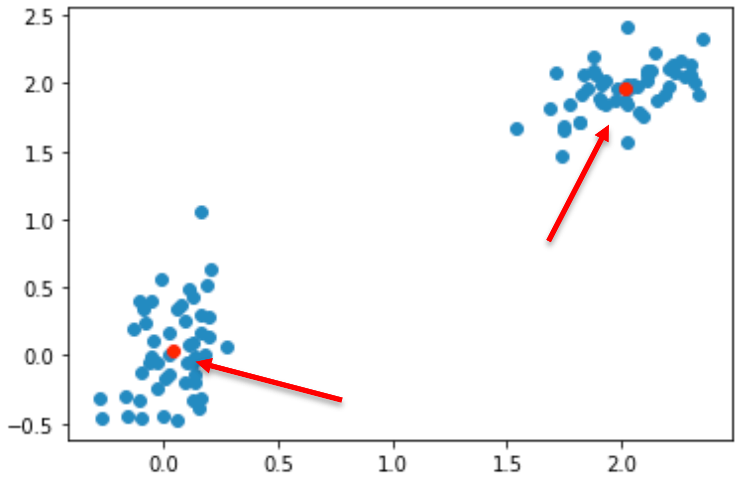
https://docs.scipy.org/doc/scipy/reference/tutorial/integrate.html

# *scipy.clustering*

Assorted functions for inferring latent structures in data, *e.g. k-means, vector-quantization, hierarchical clustering*

```
>>> import numpy as np
>>> from scipy.cluster.vq import vq, kmeans, whiten
>>> import matplotlib.pyplot as plt
>>> # 50 pts at (0,0)
>>> a = np.random.multivariate_normal([ 0, 0],
... [[ 4, 1], [1, 4]],
... size=50)
...
>>> # 50 pts at (30,10)
>>> b = np.random.multivariate_normal([30, 10],
... [[10, 2], [2, 1]],
... size=50)
...
>>> features = np.concatenate((a, b)) # x = [ a, b ]
>>> x = whiten(features) # normalize data
>>> y, e = kmeans(x, 2) # infer k=2 means
>>> plt.scatter(x[:, 0], x[:, 1]) # plot data, x
>>> plt.scatter(y[:, 0], y[:, 1], # plot means, y
...             c='r’)
>>> plt.show()
```

k=2 means

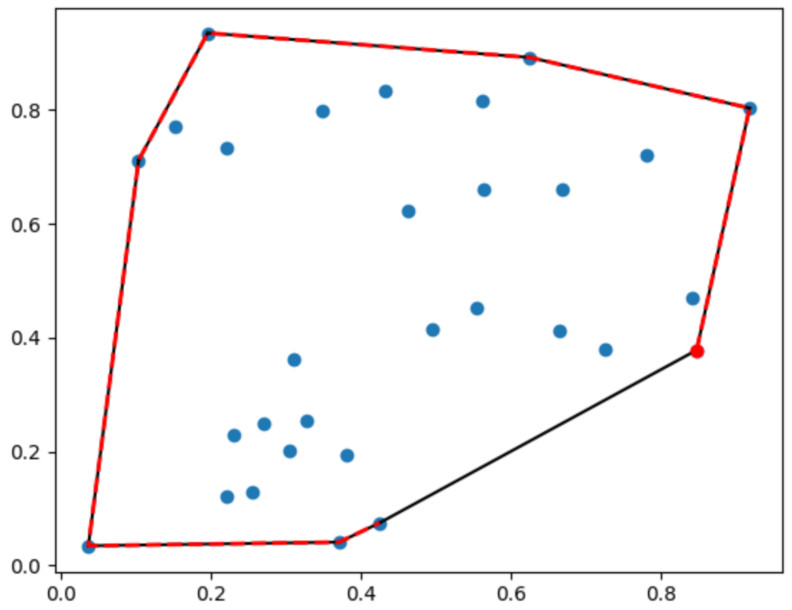


https://docs.scipy.org/doc/scipy/reference/cluster.html

# *scipy.spatial.ConvexHull*

polygons to quantify the spread/shape of data

```
>>> # import numpy/scipy
>>> import numpy as np
>>> import scipy as sp
>>> # simulate dataset
>>> np.random.seed(seed=12345)
>>> points = sp.stats.uniform.rvs(size=(30,2))
>>> # find convex hull of points
>>> hull = sp.spatial.ConvexHull(points)
>>> hull.area
3.008424594700238
>>> hull.points[hull.vertices,:]
array([[0.846943 , 0.37809954],
[0.9174485 , 0.80358537],
[0.62491062, 0.89256119],
[0.19608178, 0.9354918 ],
[0.10410446, 0.71212017],
[0.03714544, 0.03413158],
[0.37113194, 0.04055327],
[0.4249371 , 0.0743783 ]])
```



```
>>> # import numpy/scipy
>>> import matplotlib.pyplot as plt
>>> # plot raw data
>>> plt.plot(points[:,0], points[:,1], 'o’)
>>> # plot convex hull
>>> for simplex in hull.simplices:
+++     plt.plot(points[simplex, 0], points[simplex, 1], 'k-')
>>> plt.plot(points[hull.vertices,0], points[hull.vertices,1], 'r--', lw=2)
>>> plt.plot(points[hull.vertices[0],0], points[hull.vertices[0],1], 'ro')
>>> plt.show()
```

https://docs.scipy.org/doc/scipy/reference/generated/scipy.spatial.ConvexHull.html

## Overview for Lab 21