Mon, Dec 07

Lecture 13A:

Python: SciPy

Practical Bioinformatics (Biol 4220)
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Lecture 13A outline

1. Overview of SciPy
2. Survey of SciPy modules
3. Lab 13A overview

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 functions for a large number of probability distributions, along with many other 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 a random experiment -- *e.g. a coin flip*

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

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

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

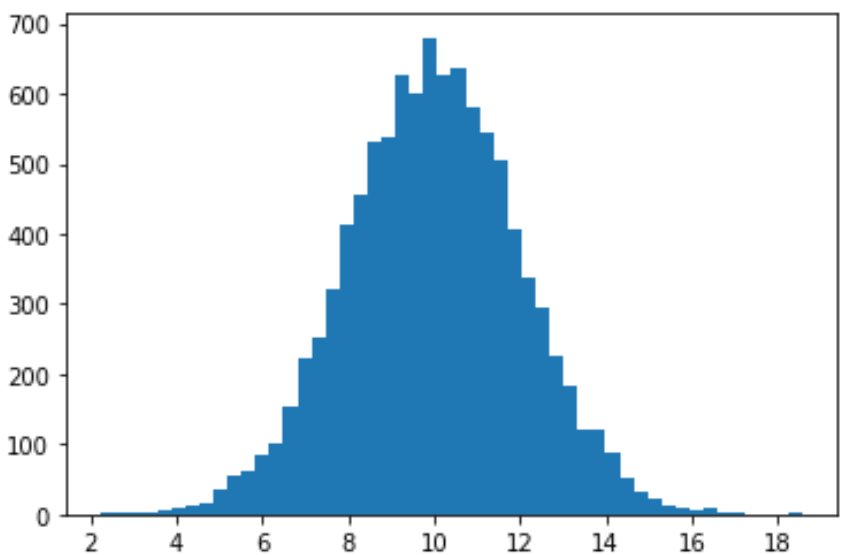
distributions in *scipy.stats*

```
>>> 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

KDEs in *scipy.stats*

Kernel density estimators (*KDEs)* approximate
a data sample 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
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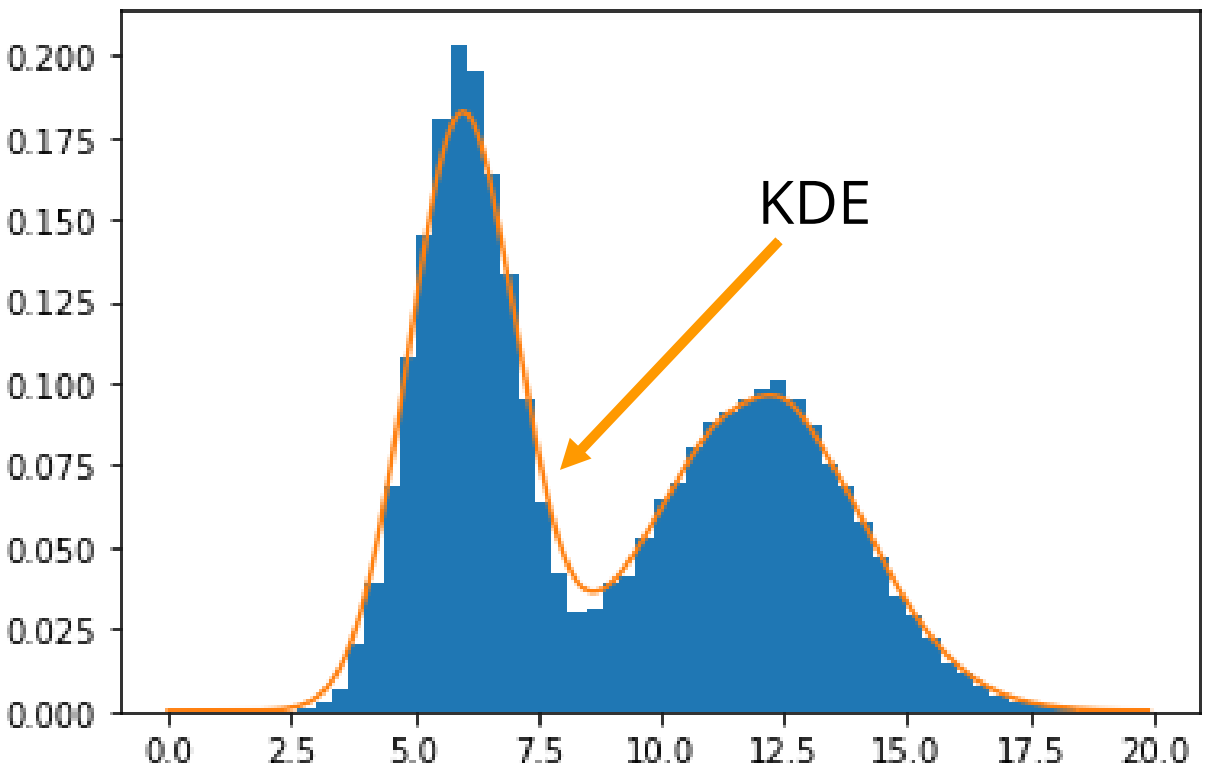
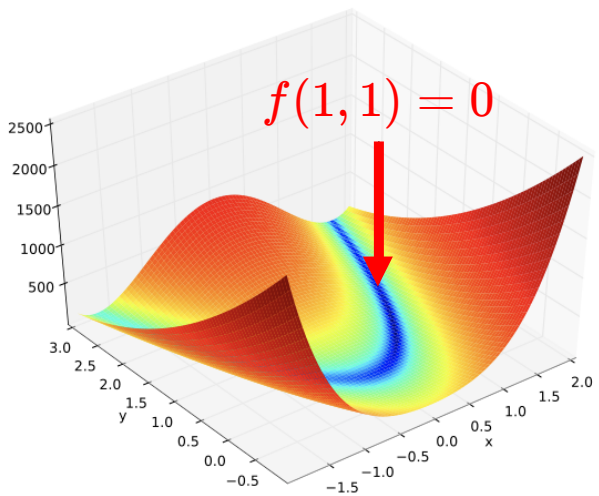


https://docs.scipy.org/doc/scipy/reference/stats.html

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
0.0
>>> rosen( [1.01, 1.01] )        # worse value
0.010300999999999994
>>> rosen( [1.05, 1.05] )        # worse value
0.2781249999999999
>>> 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
```

Methods that find arguments that maximize a user-defined function



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

$$a = 1, b = 100$$

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
```

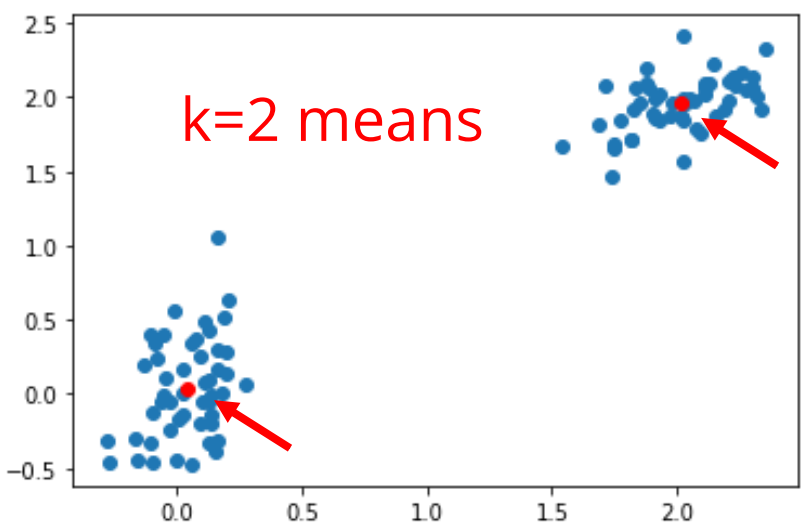
$$I = \int_0^4 x^2 dx$$
$$= F(4) - F(0)$$
$$= \frac{4^3}{3} - \frac{0^3}{3} = 21\frac{1}{3}$$

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

scipy.clustering

Various functions for inferring latent structures in data, e.g.
k-means, vector-quantization, and 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], c='r') # plot means, y
>>> plt.show()
```



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

Lab 13A

github.com/WUSTL-Biol4220/home/labs/lab_13A.md