

Lec 07 - SciPy

Statistical Computing and Computation

Sta 663 | Spring 2022

Dr. Colin Rundel

What is SciPy

Fundamental algorithms for scientific computing in Python

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

Example 1 - k-means clustering

Data

```
rng = np.random.default_rng(seed = 1234)

cl1 = rng.multivariate_normal([-2,-2], [[1,-0.5],[-0.5,1]], size=100)
cl2 = rng.multivariate_normal([1,0], [[1,0],[0,1]], size=150)
cl3 = rng.multivariate_normal([3,2], [[1,-0.7],[-0.7,1]], size=200)

pts = np.concatenate((cl1,cl2,cl3))
```

k-means clustering

```
from scipy.cluster.vq import kmeans
```

```
ctr, dist = kmeans(pts, 3)  
ctr
```

```
## array([[ 2.85409537,  1.94511779],  
##          [ 0.89789235, -0.20527898],  
##          [-2.03956666, -1.85662027]])
```

```
dist
```

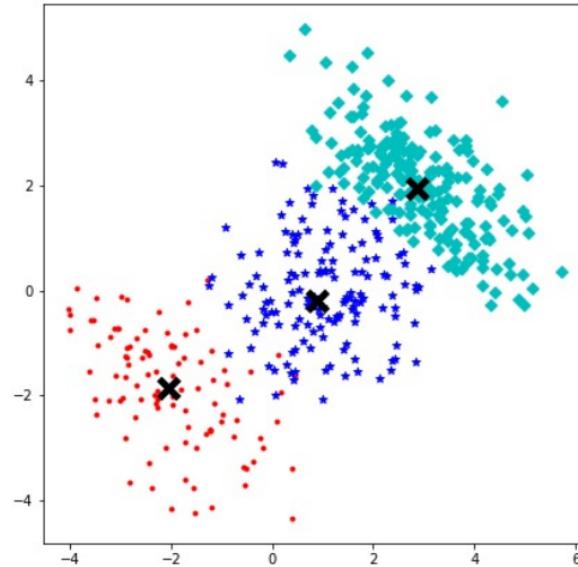
```
## 1.2206927437557962
```

```
cl1.mean(axis=0)
```

```
## array([-2.00474615, -1.87275596])
```

```
cl2.mean(axis=0)
```

```
## array([1.03849018,  0.01417119])
```



k-means distortion plot

The mean (non-squared) Euclidean distance between the observations passed and the centroids generated.

```
ks = range(1,6)
dists = [kmeans(pts, k)[1] for k in ks]

np.array(dists).reshape((-1,1))

## array([[2.5470307 ],
##        [1.57009105],
##        [1.22069274],
##        [1.04594861],
##        [0.95269843]])
```

Example 2 - Numerical integration

Basic functions

For general numeric integration in 1D we use `scipy.integrate.quad()`, which takes as arguments the function to be integrated and the lower and upper bounds of integration.

```
from scipy.integrate import quad  
  
quad(lambda x: x, 0, 1)  
  
## (0.5, 5.551115123125783e-15)  
  
quad(np.sin, 0, np.pi)  
  
## (2.0, 2.220446049250313e-14)  
  
quad(np.sin, 0, 2*np.pi)  
  
## (2.0329956258200796e-16, 4.3998892617845996e-14)  
  
quad(np.exp, 0, 1)  
  
## (1.7182818284590453, 1.9076760487502457e-14)
```

Normal PDF

The PDF for a normal distribution is given by,

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

```
def norm_pdf(x, mu, sigma):
    return (1/(sigma * np.sqrt(2*np.pi))) * np.exp(-0.5 * ((x - mu)/sigma)**2)
```

```
norm_pdf(0, 0, 1)
```

```
## 0.3989422804014327
```

```
norm_pdf(np.Inf, 0, 1)
```

```
## 0.0
```

```
norm_pdf(-np.Inf, 0, 1)
```

```
## 0.0
```

Checking the DPF

We can check that we've implemented a valid pdf by integrating the PDF from $-\infty$ to ∞ ,

```
quad(norm_pdf, -np.inf, np.inf)
```

```
## Error in py_call_impl(callable, dots$args, dots$keywords): TypeError: norm_pdf() missing 2 required positionals: 'a' and 'b'  
##  
## Detailed traceback:  
##   File "<string>", line 1, in <module>  
##   File "/opt/homebrew/lib/python3.9/site-packages/scipy/integrate/quadpack.py", line 351, in quad  
##     retval = _quad(func, a, b, args, full_output, epsabs, epsrel, limit,  
##   File "/opt/homebrew/lib/python3.9/site-packages/scipy/integrate/quadpack.py", line 465, in _quad  
##     return _quadpack._qagie(func,bound,infbounds,args,full_output,epsabs,epsrel,limit)
```

```
quad(lambda x: norm_pdf(x, 0, 1), -np.inf, np.inf)
```

```
## (0.9999999999999997, 1.0178191380347127e-08)
```

```
quad(lambda x: norm_pdf(x, 17, 12), -np.inf, np.inf)
```

```
## (1.0000000000000002, 4.113136862574909e-09)
```

Truncated normals

$$f(x) = \begin{cases} \frac{c}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right), & \text{for } a \leq x \leq b \\ 0, & \text{otherwise.} \end{cases}$$

```
def trunc_norm_pdf(x, mu=0, sigma=1, a=-np.inf, b=np.inf):
    if (b < a):
        raise ValueError("b must be greater than a")
    x = np.asarray(x).reshape(-1)
    full_pdf = (1/(sigma * np.sqrt(2*np.pi))) * np.exp(-0.5 * ((x - mu)/sigma)**2)
    full_pdf[(x < a) | (x > b)] = 0
    return full_pdf
```

Testing trunc_norm_pdf

```
trunc_norm_pdf(0, a=-1, b=1)
## array([0.39894228])

trunc_norm_pdf(2, a=-1, b=1)
## array([0.])

trunc_norm_pdf(-2, a=-1, b=1)
## array([0.])

trunc_norm_pdf([-2,1,0,1,2], a=-1, b=1)
## array([0.          , 0.24197072, 0.39894228, 0.24197072, 0.        ])

quad(lambda x: trunc_norm_pdf(x, a=-1, b=1), -np.inf, np.inf)
## (0.682689492137086, 2.0147661317082566e-11)

quad(lambda x: trunc_norm_pdf(x, a=-3, b=3), -np.inf, np.inf)
## (0.9973002039367396, 7.451935936375609e-09)
```

Fixing trunc_norm_pdf

```
def trunc_norm_pdf(x, μ=0, σ=1, a=-np.inf, b=np.inf):
    if (b < a):
        raise ValueError("b must be greater than a")
    x = np.asarray(x).reshape(-1)

    nc = 1 / quad(lambda x: norm_pdf(x, μ, σ), a, b)[0]

    full_pdf = nc * (1/(σ * np.sqrt(2*np.pi))) * np.exp(-0.5 * ((x - μ)/σ)**2)
    full_pdf[(x < a) | (x > b)] = 0

    return full_pdf
```

```
trunc_norm_pdf(0, a=-1, b=1)
```

```
## array([0.58436857])
```

```
trunc_norm_pdf(2, a=-1, b=1)
```

```
## array([0.])
```

```
trunc_norm_pdf(-2, a=-1, b=1)
```

```
## array([0.])
```

```
trunc_norm_pdf([-2,1,0,1,2], a=-1, b=1)
```

```
quad(lambda x: trunc_norm_pdf(x, a=-1, b=1), -np.inf, np.inf)
```

```
## (1.0, 2.9512170485190836e-11)
```

```
quad(lambda x: trunc_norm_pdf(x, a=-3, b=3), -np.inf, np.inf)
```

```
## (0.9999999999999998, 7.472109098127788e-09)
```

Multivariate normal

$$f(\mathbf{x}) = \det(2\pi\Sigma)^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})\right)$$

```
def mv_norm(x, mu, Sigma):
    x = np.asarray(x)
    mu = np.asarray(mu)
    Sigma = np.asarray(Sigma)

    return np.linalg.det(2*np.pi*Sigma)**(-0.5) * np.exp(-0.5 * (x - mu).T @ np.linalg.solve(Sigma, (x-mu)) )
```

```
norm_pdf(0,0,1)
## 0.3989422804014327
mv_norm([0], [0], [[1]])
## 0.3989422804014327
mv_norm([0,0], [0,0], [[1,0],[0,1]])
## 0.15915494309189535
mv_norm([0,0,0], [0,0,0], [[1,0,0],[0,1,0],[0,0,1]])
```

```
from scipy.integrate import dblquad, tplquad
dblquad(lambda y, x: mv_norm([x,y], [0,0], np.identity(2)),
        a=-np.inf, b=np.inf,
        gfun=lambda x: -np.inf, hfun=lambda x: np.inf)
## (1.000000000000322, 1.3150127836618008e-08)

tplquad(lambda z, y, x: mv_norm([x,y,z], [0,0,0], np.identity(3),
        a=0, b=np.inf,
        gfun=lambda x: 0, hfun=lambda x: np.inf,
        qfun=lambda x,y: 0, rfun=lambda x,y: np.inf)
```

Example 3 - (Very) Basic optimization

Scalar function minimization

```
def f(x):
    return x**4 + 3*(x-2)**3 - 15*(x)**2 + 1
```

```
from scipy.optimize import minimize_scalar
minimize_scalar(f, method="Brent")
```

```
##      fun: -803.3955308825884
##      nfev: 17
##      nit: 11
##  success: True
##          x: -5.528801125219663
```

```
minimize_scalar(f, method="bounded", bounds=[0, 6])
```

```
##      fun: -54.21003937712762
##  message: 'Solution found.'
##      nfev: 12
##      status: 0
##  success: True
##          x: 2.668865104039653
```

```
minimize_scalar(f, method="bounded", bounds=[-8, 6])
```

```
##      fun: -803.3955308825871
```

Results

```
res = minimize_scalar(f)

type(res)

## <class 'scipy.optimize.optimize.OptimizeResult'>

dir(res)

## ['fun', 'nfev', 'nit', 'success', 'x']

res.success

## True

res.x

## -5.528801125219663
```

More details

```
from scipy.optimize import show_options
show_options(solver="minimize_scalar")

##
## brent
## -----
##
## Options
## -----
## maxiter : int
##     Maximum number of iterations to perform.
## xtol : float
##     Relative error in solution `xopt` acceptable for convergence.
##
## Notes
## -----
## Uses inverse parabolic interpolation when possible to speed up
## convergence of golden section method.
##
## bounded
## -----
##
## Options
## -----
## maxiter : int
##     Maximum number of iterations to perform.
## disp: int, optional
##     If non-zero, print messages.
##     0 : no message printing.
```

Local minima

```
def f(x):  
    return -np.sinc(x-5)
```

```
res = minimize_scalar(f)  
res  
  
##      fun: -0.049029624014074166  
##      nfev: 15  
##      nit: 10  
##  success: True  
##            x: -1.4843871263953001
```

Random starts

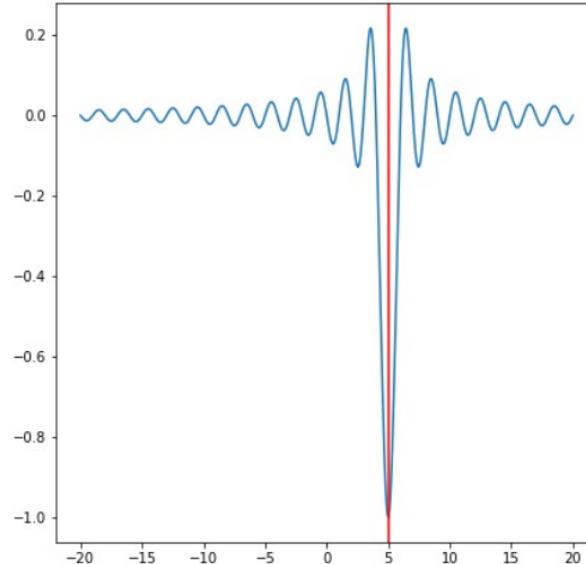
```
rng = np.random.default_rng(seed=1234)

lower = rng.uniform(-20, 20, 100)
upper = lower + 1

sols = [minimize_scalar(f, bracket=(l,u)) for l,u
        in zip(lower, upper)]
functs = [sol.fun for sol in sols]

best = sols[np.argmin(functs)]
best

##      fun: -1.0
##      nfev: 12
##      nit: 8
##  success: True
##      x: 5.000000000618556
```



Back to Rosenbrock's function

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

```
def f(x):
    return (1-x[0])**2 + 100*(x[1]-x[0]**2)**2

from scipy.optimize import minimize

minimize(f, [0,0])

##      fun: 2.844030241790906e-11
##  hess_inv: array([[0.49482454,  0.98957635],
##                  [0.98957635,  1.98394216]])
##      jac: array([-3.98673382e-06, -2.84416264e-06])
##  message: 'Optimization terminated successfully.'
##      nfev: 72
##       nit: 19
##       njev: 24
##      status: 0
##     success: True
##         x: array([0.99999467,  0.99998932])

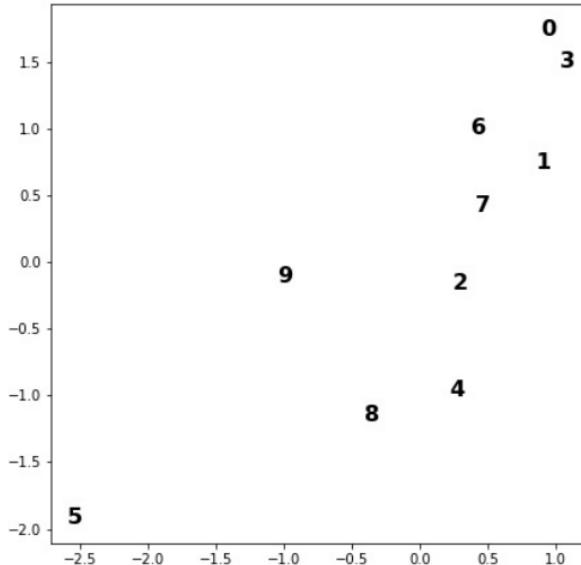
minimize(f, [-1,-1]).x
```

Example 4 - Spatial Tools

Nearest Neighbors

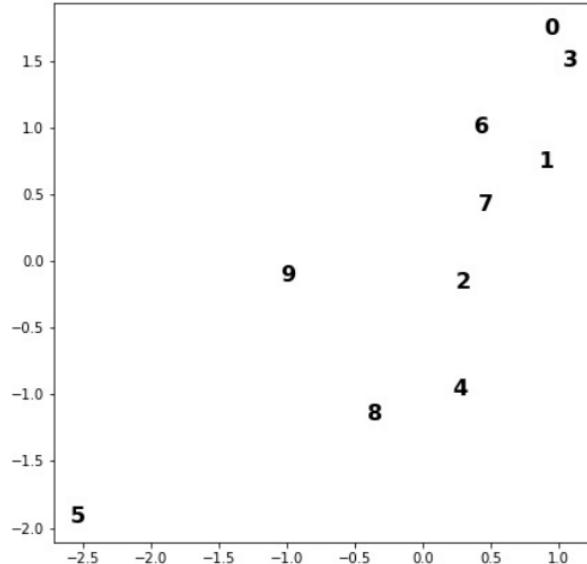
```
rng = np.random.default_rng(seed=12345)
pts = rng.multivariate_normal(
    [0,0], [[1,.8],[.8,1]],
    size=10
)

pts
## array([[ 0.951133 ,  1.75038506],
##        [ 0.90794002,  0.74402448],
##        [ 0.30576524, -0.16281136],
##        [ 1.09240417,  1.50280001],
##        [ 0.27501972, -0.96007933],
##        [-2.53321395, -1.92068272],
##        [ 0.43511779,  1.00571808],
##        [ 0.46218239,  0.42379897],
##        [-0.3509701 , -1.14575681],
##        [-0.98870241, -0.1039104 ]])
```



KD Trees

```
from scipy.spatial import KDTree  
  
kd = KDTree(pts)  
kd  
  
## <scipy.spatial.kdtree.KDTree object at 0x1026b4  
  
dir(kd)  
  
## ['__class__', '__delattr__', '__dict__', '__dir__  
  
dist, i = kd.query(pts[6,:], k=3)  
dist  
  
## array([0.           , 0.54041133, 0.58254815])  
  
i  
  
## array([6, 1, 7])  
  
dist, i = kd.query(pts[2,:], k=5)  
i
```



Convex hulls

```
from scipy.spatial import ConvexHull  
  
hull = ConvexHull(pts)  
hull  
  
## <scipy.spatial.qhull.ConvexHull object at 0x147  
  
dir(hull)  
  
## ['__class__', '__del__', '__delattr__', '__dict__  
  
hull.simplices  
  
## array([[0, 3],  
##         [4, 5],  
##         [9, 5],  
##         [9, 0],  
##         [1, 3],  
##         [1, 4]], dtype=int32)
```

```
scipy.spatial.convex_hull_plot_2d(hull)
```



Delaunay triangulations

```
from scipy.spatial import Delaunay  
  
tri = Delaunay(pts)  
tri  
  
## <scipy.spatial.qhull.Delaunay object at 0x1477a  
  
dir(tri)  
  
## ['__class__', '__del__', '__delattr__', '__dict__  
  
tri.simplices  
  
## array([[8, 9, 5],  
##         [4, 8, 5],  
##         [9, 8, 2],  
##         [8, 4, 2],  
##         [4, 1, 2],  
##         [6, 1, 3],  
##         [0, 6, 3],  
##         [6, 0, 9],  
##         [7, 9, 2],  
##         [7, 6, 9],
```

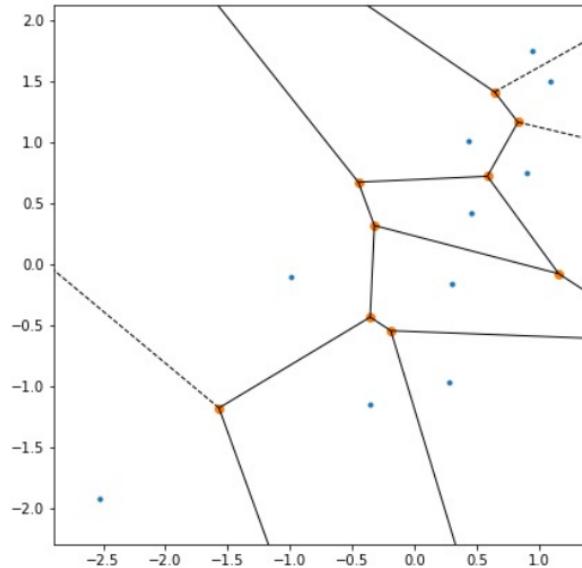
```
scipy.spatial.delaunay_plot_2d(tri)
```



Voronoi diagrams

```
from scipy.spatial import Voronoi  
  
vor = Voronoi(pts)  
vor  
  
## <scipy.spatial.qhull.Voronoi object at 0x1477c2  
  
dir(vor)  
  
## ['__class__', '__del__', '__delattr__', '__dict__  
  
vor.vertices  
  
## array([[-1.56917821, -1.17533646],  
##        [ 7.94738786, -27.97463108],  
##        [-0.3550644 , -0.43215628],  
##        [-0.18923926, -0.54294902],  
##        [ 1.98860973, -0.62693469],  
##        [ 0.83175084,  1.16435674],  
##        [ 0.64483401,  1.41151497],  
##        [-2.98645423,  3.92780753],  
##        [-0.32091034,  0.31844817],  
##        [-0.44985535,  0.67296975],  
##        [-1.5 ,  0. ]])
```

```
scipy.spatial.voronoi_plot_2d(vor)
```



Example 5 - stats

Distributions

Implements classes for 104 continuous and 19 discrete distributions,

- rvs: Random Variates
- pdf: Probability Density Function
- cdf: Cumulative Distribution Function
- sf: Survival Function (1-CDF)
- ppf: Percent Point Function (Inverse of CDF)
- isf: Inverse Survival Function (Inverse of SF)
- stats: Return mean, variance, (Fisher's) skew, or (Fisher's) kurtosis
- moment: non-central moments of the distribution

Basic usage

```
from scipy.stats import norm, gamma, binom, uniform

norm().rvs(size=5)

## array([ 1.37773488, -0.19096664,  0.55300367,  1.10696328,  0.49030573])

uniform.pdf([0,0.5,1,2])

## array([1., 1., 1., 0.])

binom.mean(n=10, p=0.25)

## 2.5

binom.median(n=10, p=0.25)

## 2.0

gamma(a=1,scale=1).stats()

## (array(1.), array(1.))

norm().stats(moments="mvsk")
```

Freezing

Model parameters can be passed to any of the methods directory, or a distribution can be constructed using a specific set of parameters, which is known as freezing.

```
norm_rv = norm(loc=-1, scale=3)
norm_rv.median()

## -1.0

unif_rv = uniform(loc=-1, scale=2)
unif_rv.cdf([-2,-1,0,1,2])

## array([0. , 0. , 0.5, 1. , 1. ])

unif_rv.rvs(5)

## array([ 0.05213907, -0.04603696,  0.29595061,
```

```
g = gamma(a=2, loc=0, scale=1.2)

x = np.linspace(0, 10, 100)
plt.plot(x, g.pdf(x), "k-")
plt.axvline(x=g.mean(), c="r")
plt.axvline(x=g.median(), c="b")
```

MLE

Maximum likelihood estimation is possible via the `fit()` method,

```
x = norm.rvs(loc=2.5, scale=2, size=1000, random_state=1234)
norm.fit(x)
```

```
## (2.5314811643075235, 1.946132398754459)
```

```
norm.fit(x, loc=2.5) # provide a guess for the parameter
```

```
## (2.5314811643075235, 1.946132398754459)
```

```
x = gamma.rvs(a=2.5, size=1000)
gamma.fit(x) # shape, loc, scale
```

```
## (2.717451544403441, -0.041437185161843526, 0.9293407167094078)
```

```
y = gamma.rvs(a=2.5, loc=-1, scale=2, size=1000)
gamma.fit(y) # shape, loc, scale
```

```
## (2.3325993640858007, -0.9659594238725819, 2.1028797903487417)
```