Lec 07 - SciPy

Statistical Computing and Computation

Sta 663 | Spring 2022

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Processing math: 8%

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
```

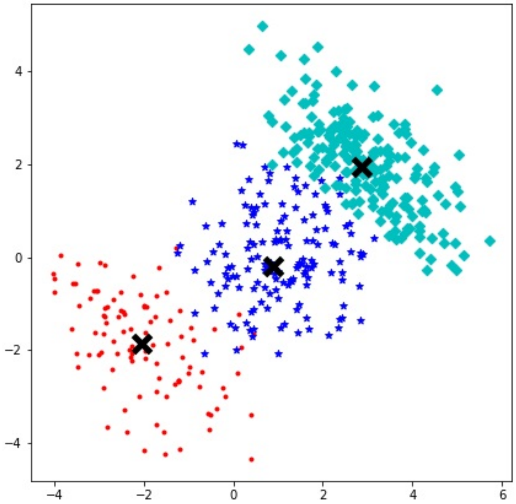
```
## 1.2206927437557962
```

```
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, μ, σ):
  return (1/(σ * np.sqrt(2*np.pi))) * np.exp(-0.5 * ((x - μ)/σ)**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 -\inf to \inf,

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

```
## Error in py_call_impl(callable, dots$args, dots$keywords): TypeError: norm_pdf() missing 2 required position
##
## 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, 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)
  full_pdf = (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
```

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

```
def mv_norm(x, μ, Σ):
  x = np.asarray(x)
  μ = np.asarray(μ)
  Σ = np.asarray(Σ)

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

```
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]])
```

```
## 0.06349363593424098
```

```
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)
```

```
## (1.0000000000000322, 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)
```

```
## (0.12500000000036066, 1.4697203688867502e-08)
```

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: -803.395530825871
```

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

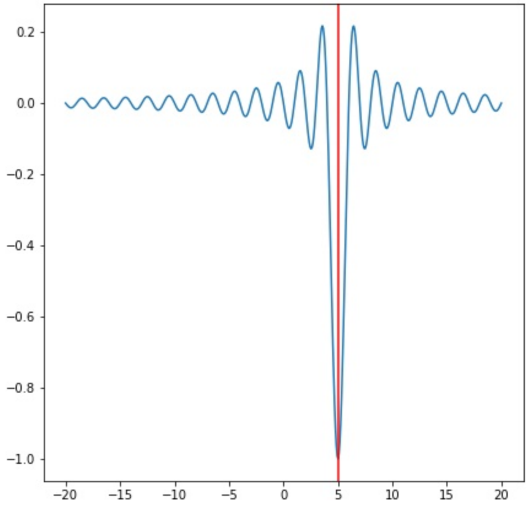
```
rng = np.random.default_rng(seed=1234)

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

sols = [minimize_scalar(f, bracket=(l,u)) for l,u
funs = [sol.fun for sol in sols]

best = sols[np.argmin(funs)]
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
```

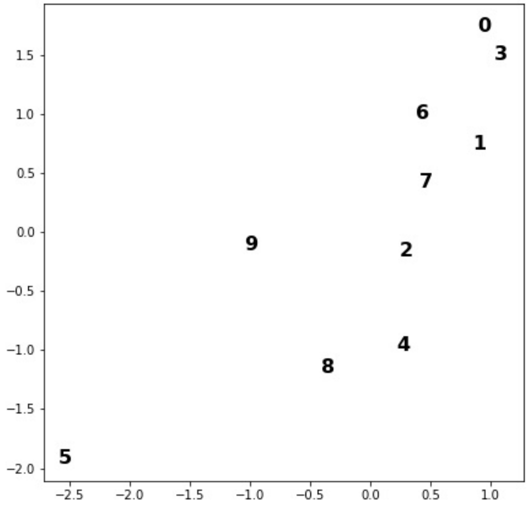
Example 4 - Spatial Tools

Nearest Neighbors

```python
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
```

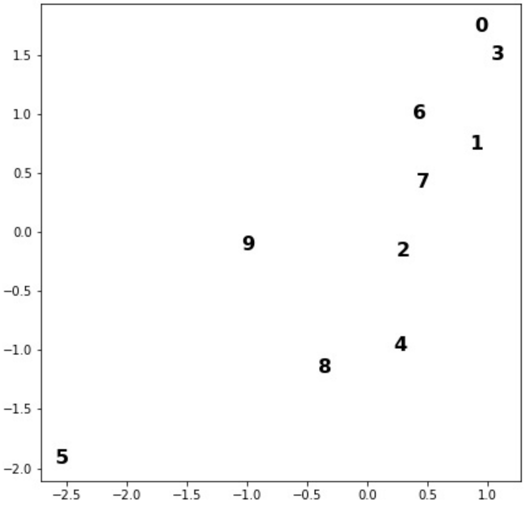
```
dist, i = kd.query(pts[6,:], k=3)
dist
```

```
## 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
```

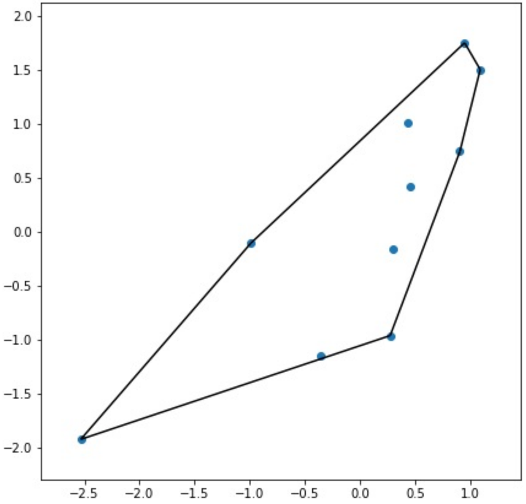
```
dir(hull)
```

```
## ['__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
```

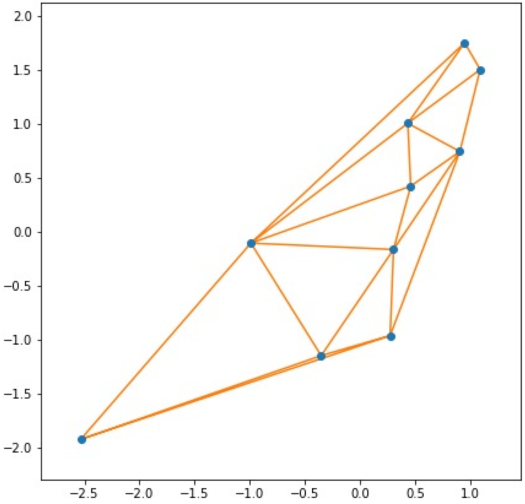
```
dir(tri)
```

```
## ['__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

```python
from scipy.spatial import Voronoi

vor = Voronoi(pts)
vor
```

```
## <scipy.spatial.qhull.Voronoi object at 0x1477c2
```

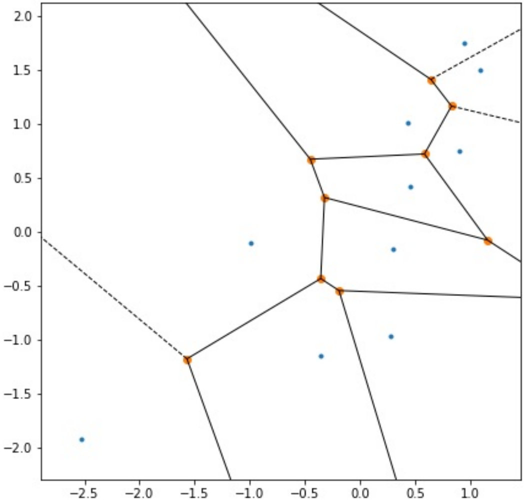
```python
dir(vor)
```

```
## ['__class__', '__del__', '__delattr__', '__dict
```

```python
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],
```

```python
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)
```