SciPy

Lecture 07

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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		

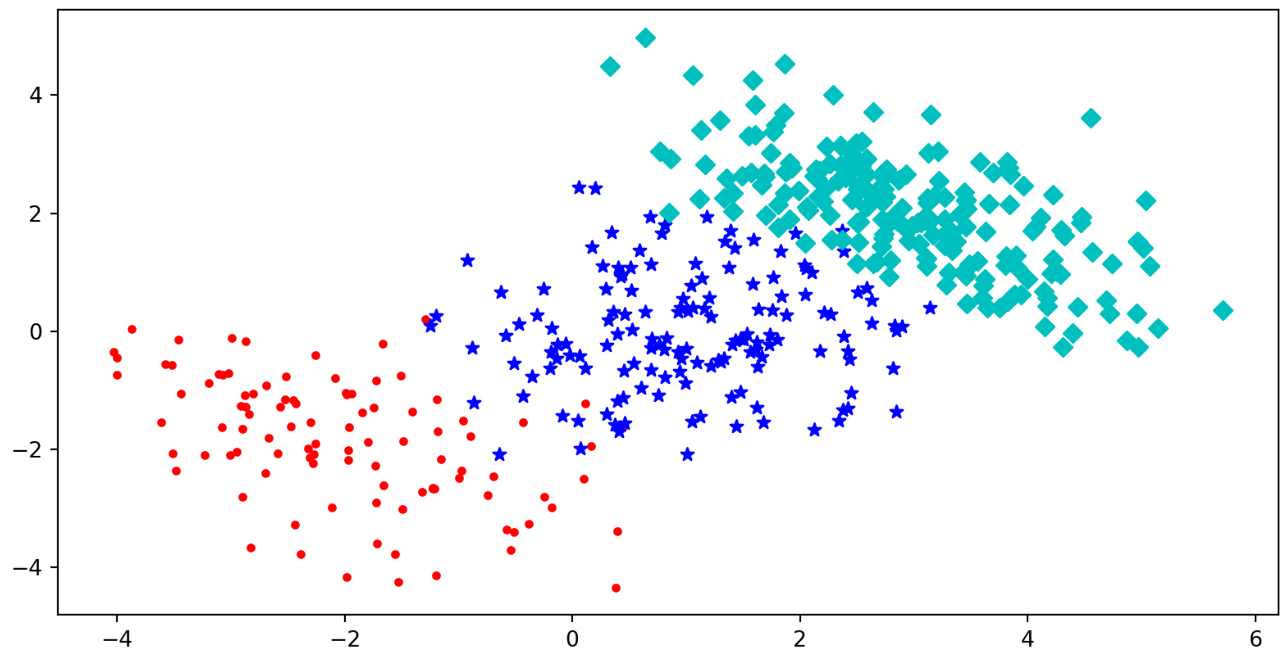
Example 1
k-means clustering

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([[ 0.8979, -0.2053],
       [ 2.8541,  1.9451],
       [-2.0396, -1.8566]])
```

```
dist
```

```
1.2206927437557962
```

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

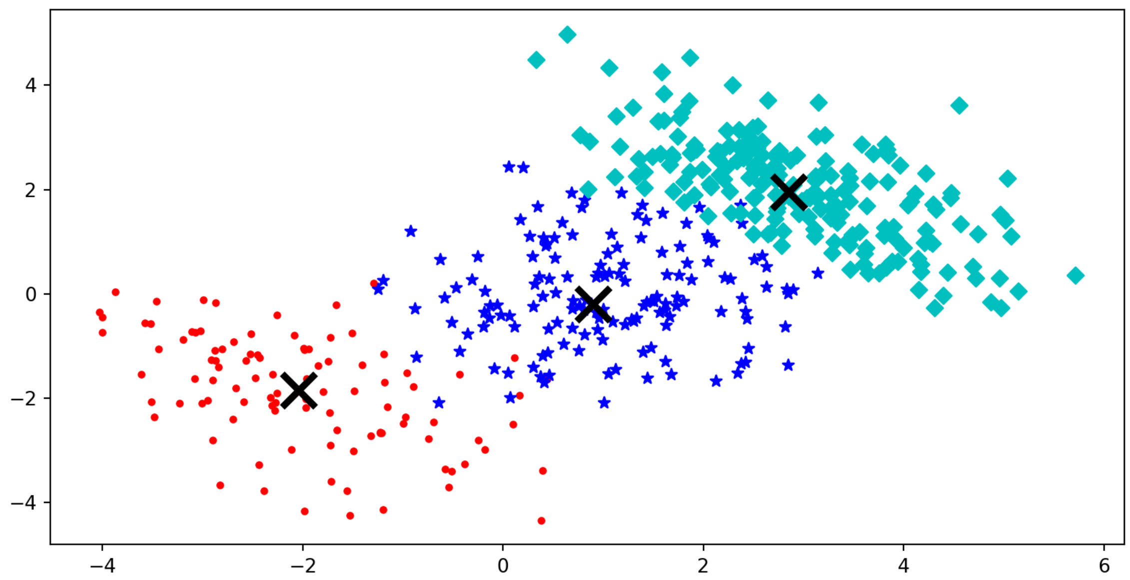
```
array([-2.0047, -1.8728])
```

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

```
array([1.0385, 0.0142])
```

```
cl3.mean(axis=0)
```

```
array([2.9464, 2.0251])
```


4
2
0
−2
−4
−4
−2
0
2
4
6

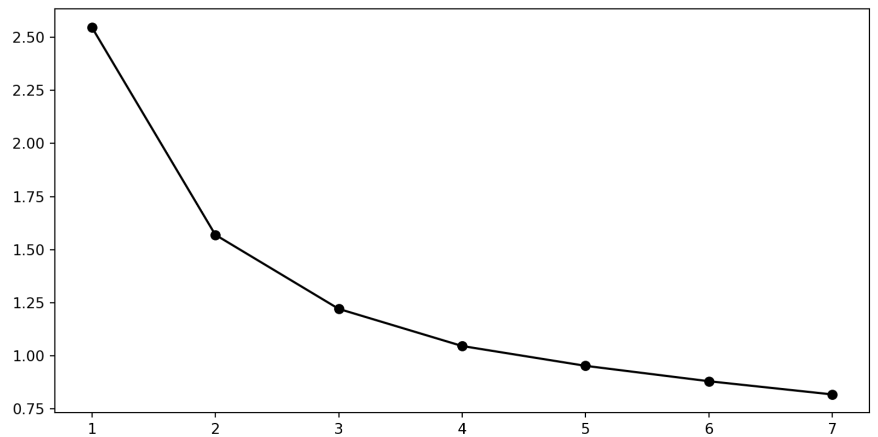
k-means distortion plot

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

```
ks = range(1,8)
dists = [kmeans(pts, k)[1] for k in ks]

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

```
array([2.547 , 1.5699, 1.2209, 1.046 , 0.9527, 0.8801, 0.818 ])
```



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 PDF

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: TypeError: norm_pdf() missing 2 required positional arguments: 'μ' and
'σ'
```

```
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 normal PDF

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

```
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([0.3989])
```

```
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.    , 0.242 , 0.3989, 0.242 , 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([0.5844])
```

```
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.    , 0.3544, 0.5844, 0.3544, 0.    ])
```

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

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

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

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

Multivariate normal

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

```
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], [0,0], [[1,0],[0,1]])
```

```
0.15915494309189535
```

```
mv_norm([0], [0], [[1]])
```

```
0.3989422804014327
```

```
mv_norm([0,0,0], [0,0,0], [[1,0,0],[0,1,0],[0,0,
```

```
0.06349363593424098
```

2d & 3d numerical integration

are supported by `dblquad()` and `tplquad()` respectively (see `nquad()` for higher dimensions)

```
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, 1.3150127836061 5e-08)
```

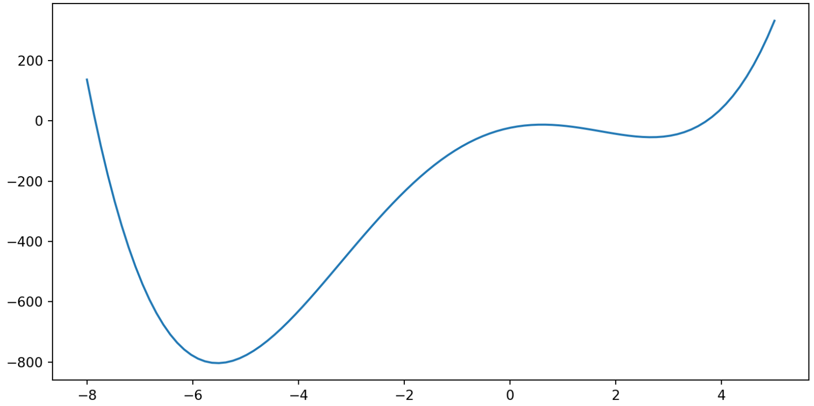
```
tplquad(lambda z, y, x: mv_norm([x,y,z], [0,0,0], np.identity(3)),
        a=0, b=np.inf,
        gfun=lambda x:   0, hfun=lambda x:   np.inf,
        qfun=lambda x,y: 0, rfun=lambda x,y: np.inf)
```

```
(0.1250000000036066, 1.4697203688867502e-08)
```

Example 3
(Very) Basic optimization

Scalar function minimization

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




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

```
 message: 
          Optimization terminated successfully;
          The returned value satisfies the termination criteria
          (using xtol = 1.48e-08 )
 success: True
     fun: -803.3955308825884
       x: -5.528801125219663
     nit: 11
    nfev: 16
```

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

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

```python
minimize_scalar(f, method="bounded", bounds=[-8,
```

```
 message: Solution found.
 success: True
  status: 0
     fun: -803.3955308825871
       x: -5.528801009134004
     nit: 12
    nfev: 12
```

Results

```
res = minimize_scalar(f)
type(res)
```

```
<class 'scipy.optimize._optimize.OptimizeResult'>
```

```
dir(res)
```

```
['fun', 'message', 'nfev', 'nit', 'success', 'x']
```

```
res.success
```

```
True
```

```
res.x
```

```
-5.52880125219663
```

More details

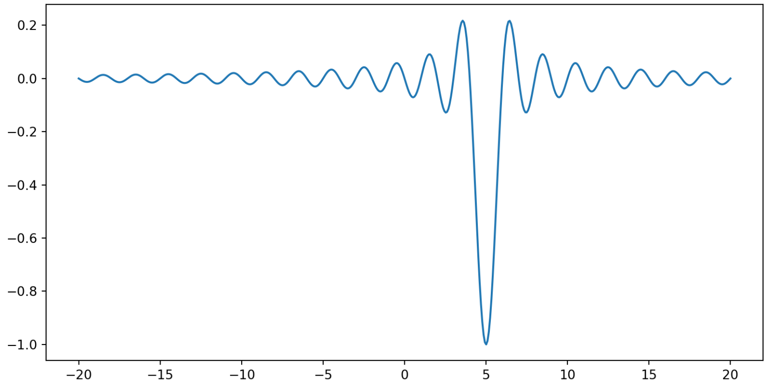
```python
from scipy.optimize import show_options
show_options(solver="minimize_scalar")
```

```
brent
=====

Options
-------
maxiter : int
    Maximum number of iterations to perform.
xtol : float
    Relative error in solution `xopt` acceptable for convergence.
disp: int, optional
    If non-zero, print messages.
        0 : no message printing.
        1 : non-convergence notification messages only.
        2 : print a message on convergence too.
        3 : print iteration results.
```

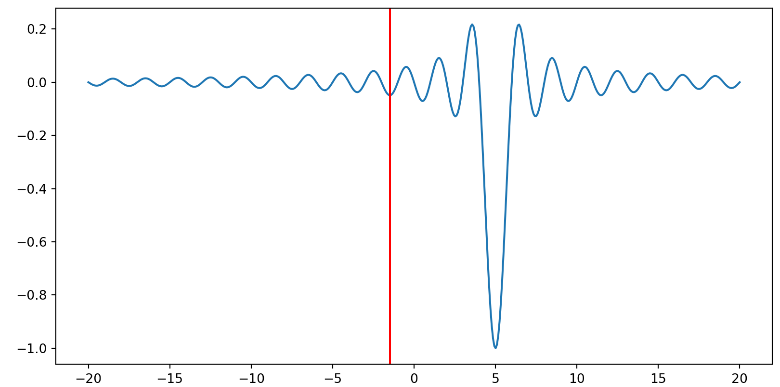
Local minima

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




```python
res = minimize_scalar(f); res
```

```
 message: 
          Optimization terminated successfully;
          The returned value satisfies the
termination criteria
          (using xtol = 1.48e-08 )
 success: True
     fun: -0.049029624014074166
       x: -1.4843871263953001
     nit: 10
    nfev: 14
```



Random starts

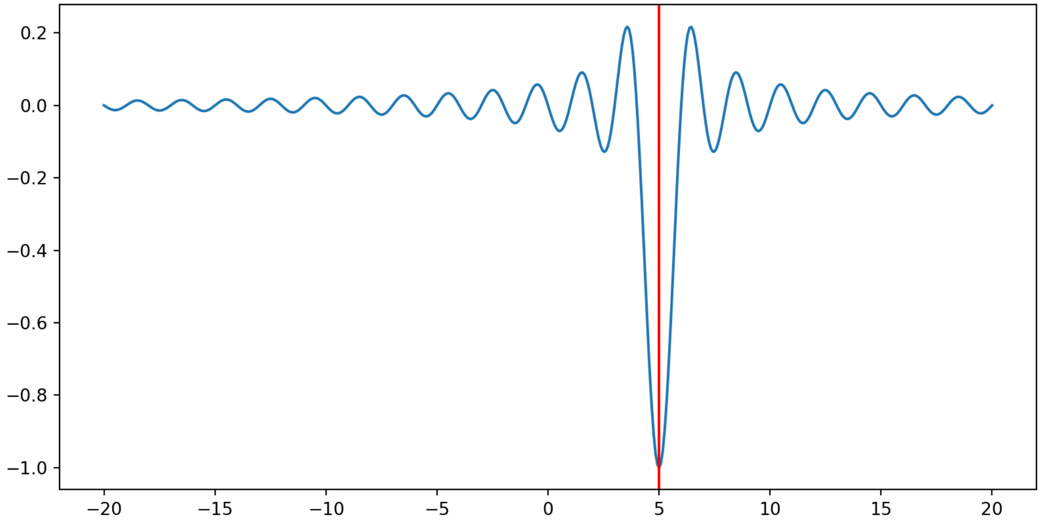
```
rng = np.random.default_rng(seed=1234)

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

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

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

```
 message:
          Optimization terminated successfully;
          The returned value satisfies the
termination criteria
          (using xtol = 1.48e-08 )
 success: True
     fun: -1.0
       x: 5.000000000618556
     nit: 8
    nfev: 11
```



Back to Rosenbrock's function

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

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

```python
minimize(f, [0,0])
```

```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: 2.843987518235081e-11
       x: [ 1.000e+00  1.000e+00]
     nit: 19
     jac: [ 3.987e-06 -2.844e-06]
hess_inv: [[ 4.948e-01  9.896e-01]
           [ 9.896e-01  1.984e+00]]
    nfev: 72
    njev: 24
```

```python
minimize(f, [-1,-1])
```

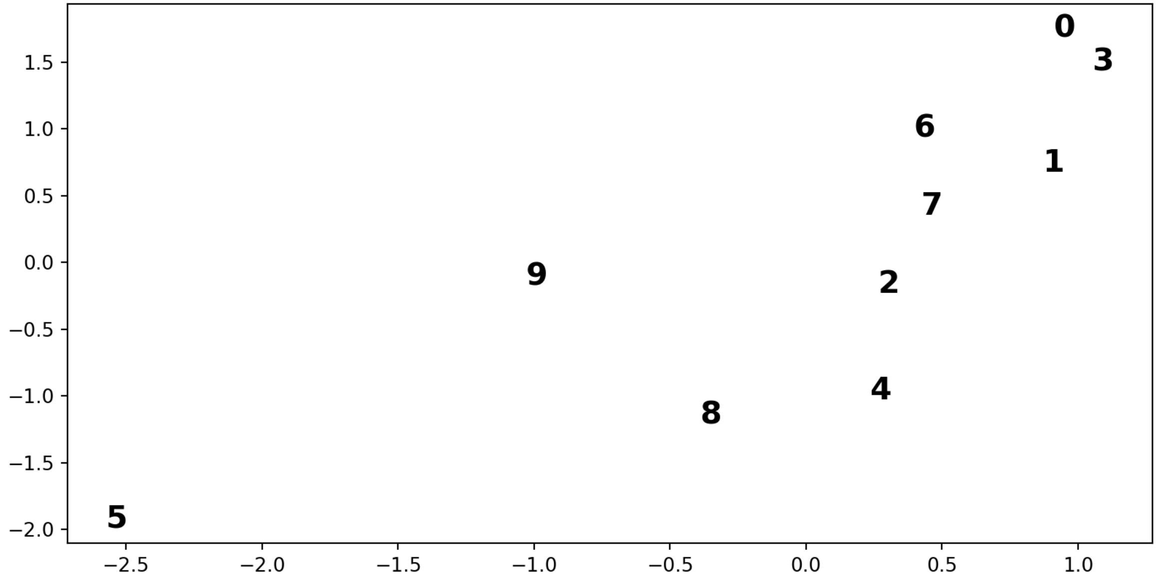
```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: 1.9950032694539075e-11
       x: [ 1.000e+00  1.000e+00]
     nit: 31
     jac: [ 2.789e-07 -1.275e-07]
hess_inv: [[ 5.085e-01  1.016e+00]
           [ 1.016e+00  2.037e+00]]
    nfev: 120
    njev: 40
```

Example 4
Spatial Tools

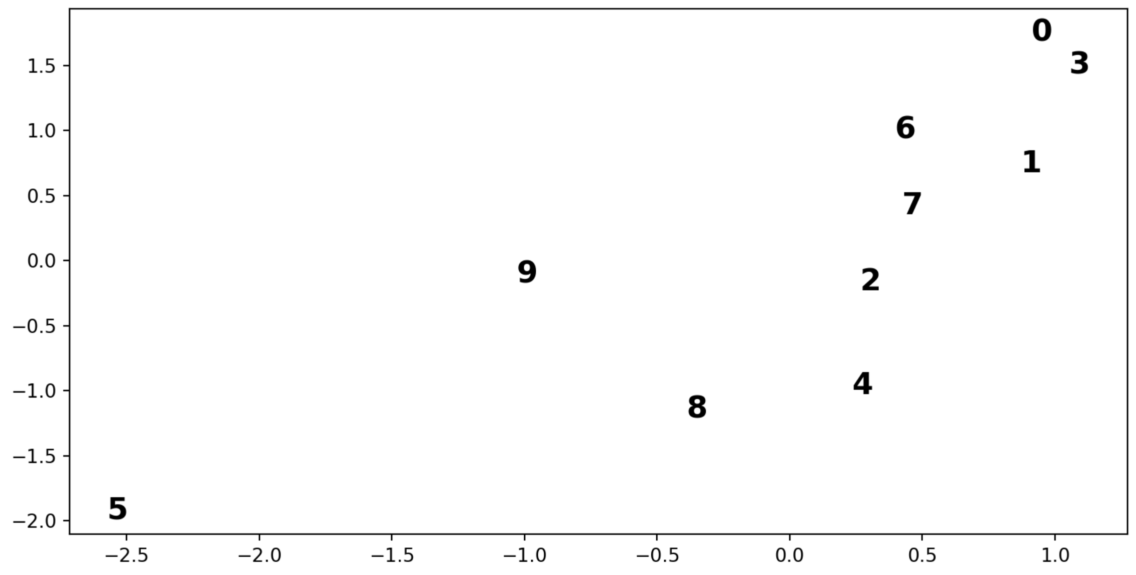
Nearest Neighbors

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

```
array([[ 0.9511,  1.7504],
       [ 0.9079,  0.744 ],
       [ 0.3058, -0.1628],
       [ 1.0924,  1.5028],
       [ 0.275 , -0.9601],
       [-2.5332, -1.9207],
       [ 0.4351,  1.0057],
       [ 0.4622,  0.4238],
       [-0.351 , -1.1458],
       [-0.9887, -0.1039]])
```



KD Trees




```python
from scipy.spatial import KDTree
kd = KDTree(pts)
```

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

```
array([6, 1, 7])
```

```python
dist
```

```
array([0.    , 0.5404, 0.5825])
```

```python
dist, i = kd.query(pts[2,:], k=5)
i
```

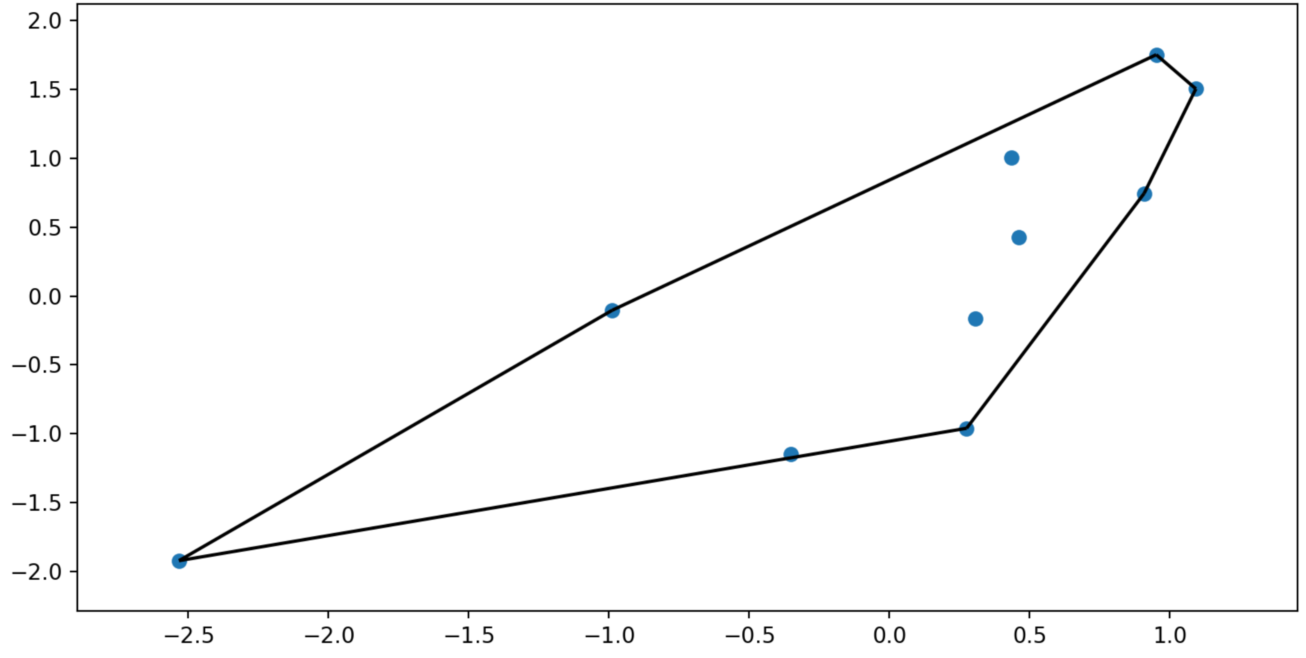
```
array([2, 7, 4, 1, 6])
```

Convex hulls

```
from scipy.spatial import ConvexHull
hull = ConvexHull(pts)
hull.vertices
```

```
array([3, 0, 9, 5, 4, 1], dtype=int32)
```

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

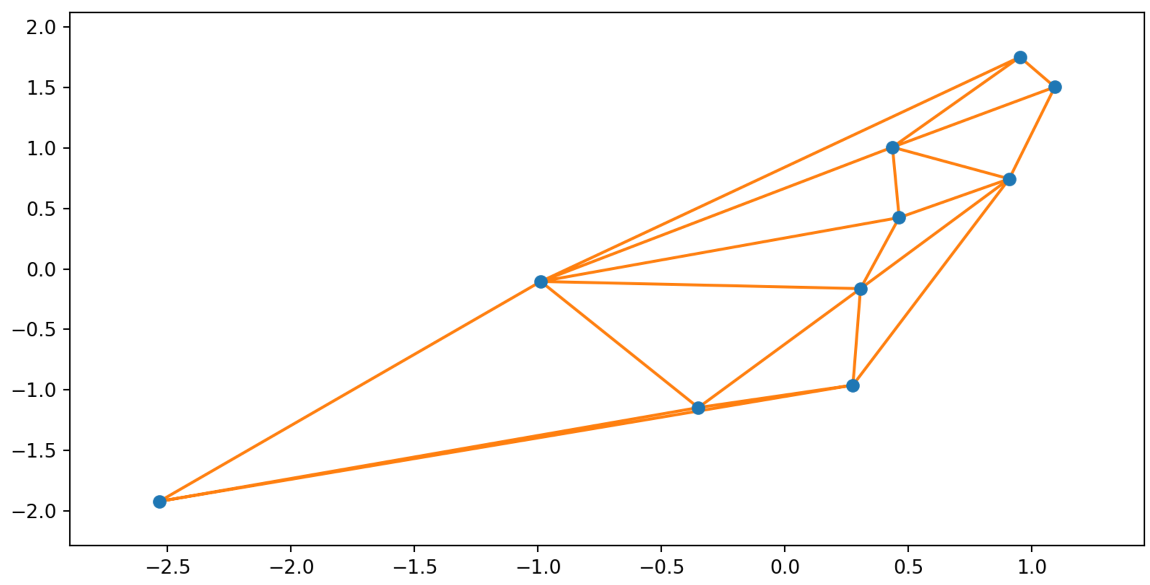


Delaunay triangulations

```python
from scipy.spatial import Delaunay
tri = Delaunay(pts)
tri.simplices.T
```

```
array([[8, 4, 9, 8, 4, 6, 0, 6, 7, 7, 1, 7],
       [9, 8, 8, 4, 1, 1, 6, 0, 9, 6, 7, 1],
       [5, 5, 2, 2, 2, 3, 3, 9, 2, 9, 2, 6]], dtype=int32)
```

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

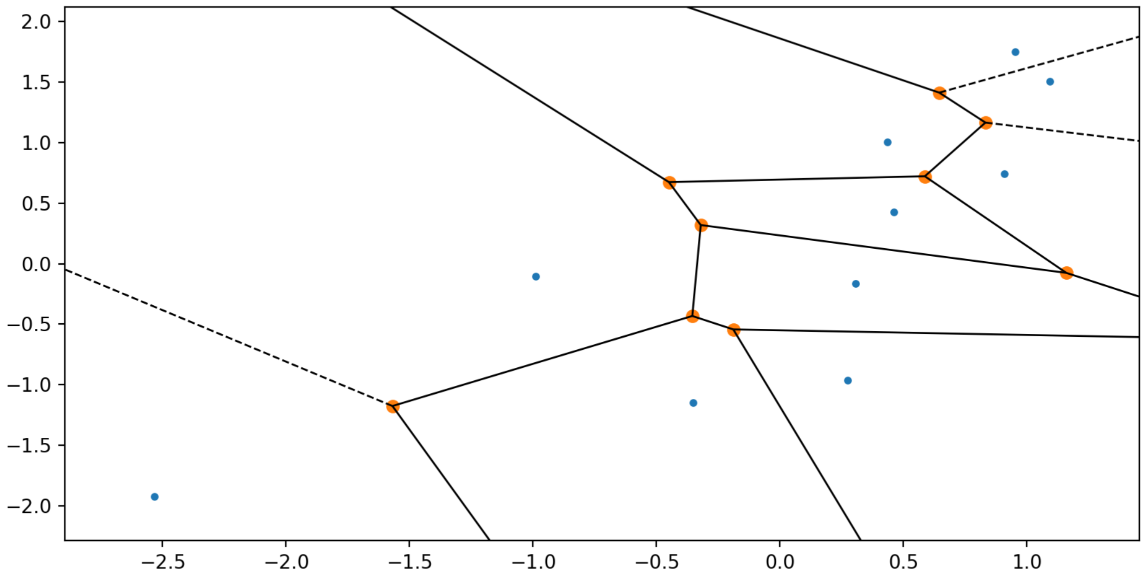


Voronoi diagrams

```
from scipy.spatial import Voronoi
vor = Voronoi(pts)
vor.vertices.T
```

```
array([[ -1.5692,   7.9474,  -0.3551,  -0.1892,   1.9886,   0.8318,   0.6448,  -2.9865,  -0.3209,
-0.4499,   1.1593,   0.5865],
       [ -1.1753, -27.9746,  -0.4322,  -0.5429,  -0.6269,   1.1644,   1.4115,   3.9278,   0.3184,   0.673
,  -0.0762,   0.7212]])
```

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



Example 5
statistics

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

```python
from scipy.stats import norm, gamma, binom, uniform
norm().rvs(size=5)
```

```
array([-0.1844, -0.3056, -0.6316,  2.0088,  1.1439])
```

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

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

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

```
2.5
```

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

```
2.0
```

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

```
(1.0, 1.0)
```

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

```
(0.0, 1.0, 0.0, 0.0)
```

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])
```

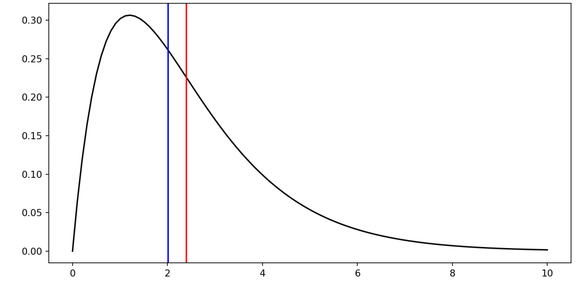
```
array([0. , 0. , 0.5, 1. , 1. ])
```

```
unif_rv.rvs(5)
```

```
array([ 0.8658, -0.2719,  0.9381,
0.8072,  0.6935])
```

```
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
```

```
(2.524523021224041 5, 0.008858045832099148, 0.9936721955371237)
```

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

```
(2.516056504365961 3, -1.011774108774102 1, 1.986807160280627 6)
```