

Data Sciences using Python (05101305)

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CHAPTER-4

Scientific computing with Python (scipy)





Introduction of scipy

- Scipy stand as scientific computing with python. It's a open source library for computing mathematical based operation which is not possible using numpy.
- Scipy is normally use for data science and data analytics based calculation.
- Scipy distributed under BSD license library.
- is pronounced as **Sigh pi**, and it depends on the Numpy, including the appropriate and fast N-dimension array manipulation.
- It provide many numerical integration based function for scientific calculation.
- It support integration, gradient optimization, special functions, ordinary differential equation solvers, parallel programming tools, and many more.
- Why scipy and why not numpy?





Installation of scipy

- Installing scipy using pip pip install scipy
- Installing scipy using anaconda
 - install anaconda first in you machine
 - open anaconda command prompt and enter below command
 - conda install -c anaconda scipy (wait for some time package are going to download)
- Installing scipy in macos
 - sudo port install py35-numpy py35-scipy py35-matplotlib py35ipython +notebook py35-pandas py35-sympy py35-nose
 - ** For more about installation:

https://www.javatpoint.com/scipy-installation

https://www.guru99.com/scipy-tutorial.html#4





Why scipy?

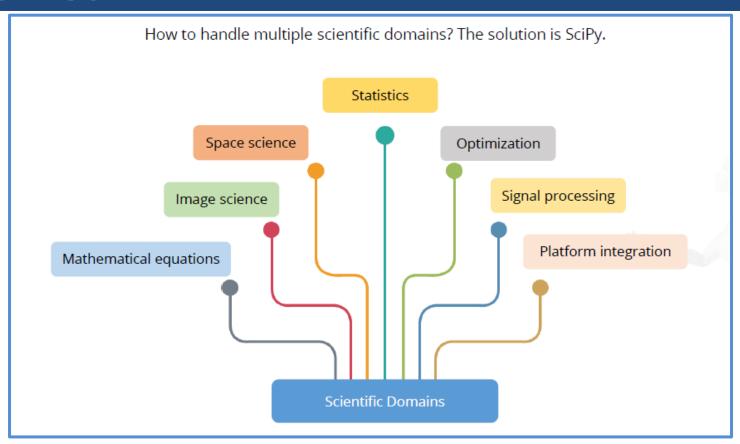
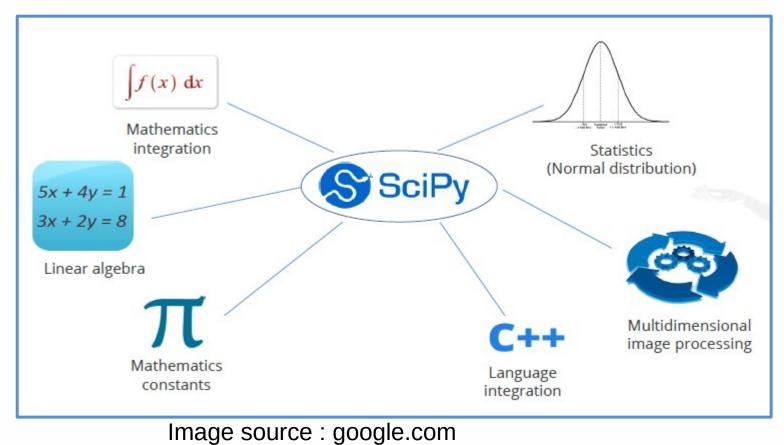


Image source : Simplilearn





Scipy have many inbuilt sub packages which is use handle to integration problem, algebraic problem, statistics and many more problem.









Characteristics of scipy

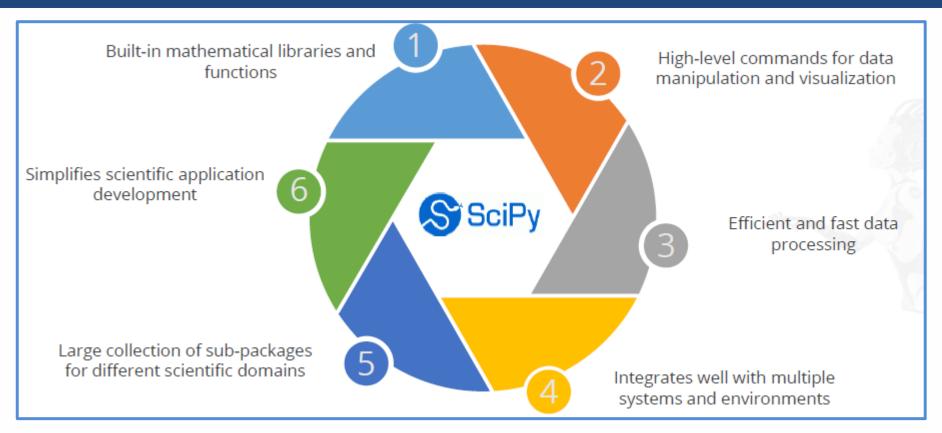


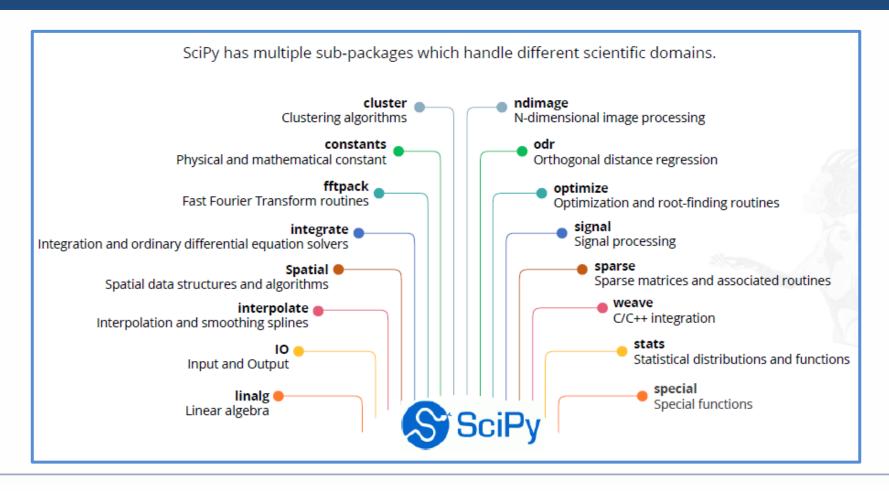
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Sub-packages of scipy

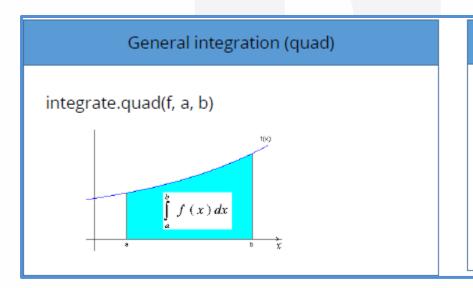






Scipy subpackage - Integration

- The **scipy.integrate** sub-package provides a number of integration techniques including an ordinary differential equation integrator.
- Which is use to solve mathematical sequences and series, or perform function approximation.



General multiple integration (dblquad, tplquad, nquad)

- integrate.dblquad()
- · integrate.tplquad()
- integrate.nquad()

The limits of all inner integrals need to be defined as functions.





Single Integrals

For single integrals quad() function is use.

Syntax : scipy.integrate.quad(f,a,b)

Where,

F is: function name for integration (user defined or inbuilt function)

A is : upper limit (numeric value)
B is : lower limit (numeric value)

• It provided to integrate a function of one variable between two points (upper limit and lower limit). The points can be $\pm\infty$ (inf) to indicate infinite limits. For example, suppose you wish to integrate a bessel function jv(2.5, x) along the interval [0,4.5] than.

$$I = \int_{0}^{4.5} J_{2.5} \left(x
ight) \, dx.$$







```
In [2]: import scipy.integrate as integrate
    import scipy.special as special
    #here we are creatig lambda function
    result = integrate.quad(lambda x: special.jv(2.5,x), 0, 4.5)
    print("value of rasult is: ",result)

    value of rasult is: (1.1178179380783244, 7.866317216380707e-09)

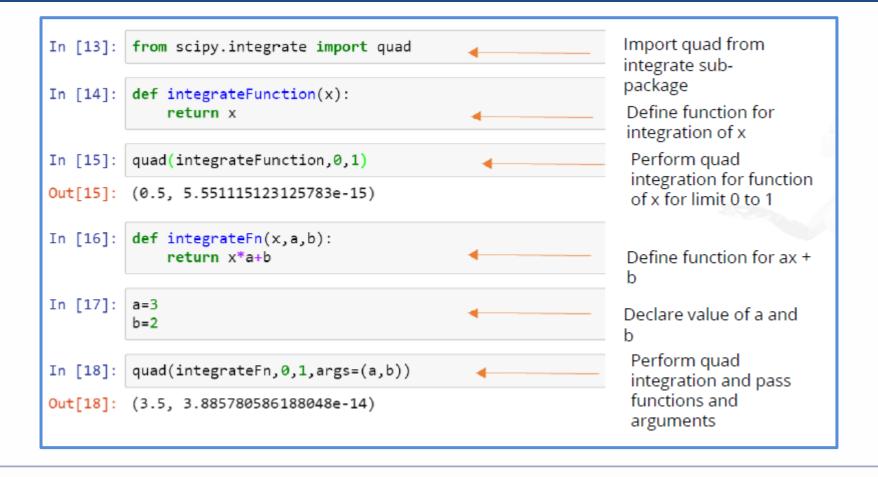
In [7]: from scipy.integrate import quad
    def integrand(x, a, b): #UDF function for ax2 + b
        return a*x**2 + b
    a = 2
    b = 1
    ans = quad(integrand, 0, 1, args=(a,b))
    print("answer is: ",ans)

    answer is: (1.6666666666666667, 1.8503717077085944e-14)
```













Multiple integration

- Is use to find double and triple integration.
- Which is rapped within the dblquad, tplquad and nquad function.
- Here dblquad() is use for double integration.
- tplquad() is use for triple integration
- nquad() use for n integration.
- For double integration
- Syntax : scipy.integrate.dblquad(func,a,b,gfun,hfun)
- Where
- Func: name of function
- a and b are upper and lower limit
- gfun and hfun are names of the functions that define the lower and upper limit of the y variable



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```
In [8]: #double integration using dblquad() function
import scipy.integrate
from numpy import exp
from math import sqrt
f = lambda x, y: 16*x*y
g = lambda x: 0
h = lambda y: sqrt(1-4*y**2)
i = scipy.integrate.dblquad(f, 0, 0.5, g, h)
print(i)

(0.5, 1.7092350012594845e-14)

In [9]: from scipy.integrate import dblquad
area = dblquad(lambda x, y: x*y, 0, 0.5, lambda x: 0, lambda x: 1-2*x)
print(area)

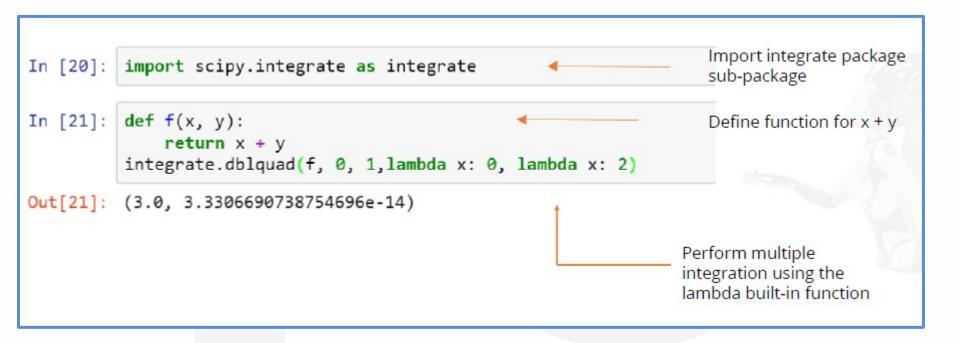
(0.0104166666666666668, 4.101620128472366e-16)
```

$$I = \int_{y=0}^{1/2} \int_{x=0}^{1-2y} xy \, dx \, dy = rac{1}{96}.$$













Scipy package optimization

- Is use to optimize or improve the performance of system mathematically by using some optimize algorithms.
- For optimizing scipy provides the list of algorithms like bfgs, Nelder-Mead simplex, Newton Conjugate Gradient, COBYLA, or SLSQP and many more.
- Is use for minimization of curve fitting, multidimensional or scalar and root fitting.
- For more please refer

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

https://www.javatpoint.com/scipy-optimize

https://www.tutorialspoint.com/scipy/scipy_optimize.htm





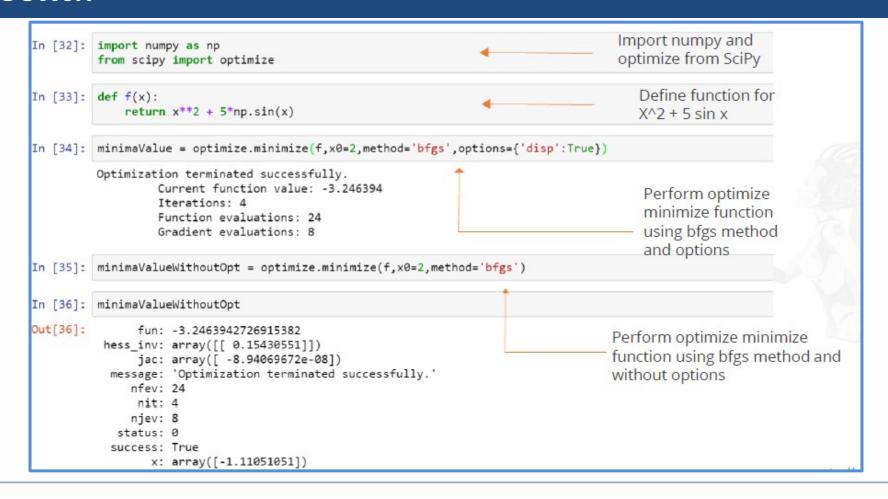
Nelder- Mead Simplex Algorithm

```
In [10]: #Nelder- Mead Simplex Algorithm
         #pvoide minimum() function
         #used for minimization of scalar function of one or more variable
         import numpy as np
         import scipy
         from scipy.optimize import minimize
         #define function f(x)
         def f(x):
            return .2*(1 - x[0])**2
         scipy.optimize.minimize(f, [2, -1], method="Nelder-Mead")
Out[10]: final_simplex: (array([[ 1. , -1.27109375],
                [ 1. , -1.27118835],
                           , -1.27113762]]), array([0., 0., 0.]))
                    fun: 0.0
                message: 'Optimization terminated successfully.'
                   nfev: 147
                    nit: 69
                 status: 0
                success: True
                     x: array([ 1. , -1.27109375])
```















Root finding

```
In [11]: #root() function is used to find the root of the nonlinear equation
         #various methods such as hybr (the default) and
         #the Levenberg-Marquardt method from the MINPACK
         import numpy as np
         from scipy.optimize import root
         def func(x):
            return x*2 + 3* np.cos(x)
         a = root(func, 0.3)
         print(a)
             fjac: array([[-1.]])
              fun: array([2.22044605e-16])
          message: 'The solution converged.'
             nfev: 10
              qtf: array([-8.13081602e-10])
                r: array([-4.37742668])
           status: 1
          success: True
                x: array([-0.91485648])
```







```
In [118]:
          import numpy as np
           from scipy.optimize import root
                                                                     Define function for
           def rootfunc(x):
                                                                     X + 3.5 \cos x
               return x + 3.5 * np.cos(x)
                                                                  Pass x value in argument for
In [119]: rootValue = root(rootfunc, 0.3)
                                                                  root
In [120]: rootValue
Out[120]:
              fjac: array([[-1.]])
                fun: array([ 2.22044605e-16])
                                                                     Function value and array
            message: 'The solution converged.'
                                                                     values
               nfev: 14
                qtf: array([ -8.32889313e-13])
                  r: array([-4.28198145])
             status: 1
            success: True
                  x: array([-1.21597614])
```





SciPy: Linear Algebra

- As scipy is handy package to perfrom datascience based computation it provide lot many functions to perform mathematical calculation.
- Scipy linear algebra provide one more package named as scipy.linalg for machine learning.
- It have advance algebraic function which working with machine learning concept.
- The ATLAS LAPACK and BLAS library, provides very fast linear algebra capabilities. Linear algebra accepts 2D array object and Gives output in 2D array object.
- Linear algebra solve given equation using the **solve()** method. Which gives result in the form of 2D array.
- The algebraic equation are in the following format
- ax+by = c for the x and y are unknown value







Solving linear equation

```
In [13]: #lets solve below given lenear equation
         #1. x + 3y + 10z = 10, 2x + 12y + 7z = 18, 5x + 8y + 8z = 30
         #let's create array for these equation
         import numpy as np
         from scipy import linalg
         coeff_arr = np.array([[1, 3, 10], [2, 12, 7], [5, 8, 8]])
         sol arr= np.array([[10], [18], [30]])
         # Solve the linear algebra
         ans = linalg.solve(coeff arr, sol arr)
         print("result is : ",ans)
         # Checking Results
         print("\n Checking results, Vectors must be zeros")
         print(coeff arr.dot(ans)-sol arr)
         result is : [[4.55393586]
          [0.51311953]
          [0.39067055]]
          Checking results, Vectors must be zeros
         [[1.77635684e-15]
          [0.00000000e+00]
          [0.00000000e+00]]
```





One more example

Linear equations

$$2x + 3y + z = 21$$

 $-x + 5y + 4z = 9$
 $3x + 2y + 9z = 6$

```
In [89]:
```

```
In [88]:
         import numpy as np
                                             Import linalg
         from scipy import linalg ←
         numArray = np.array([[2,3,1],[-1,5,4],[3,2,9]])
In [90]: numArrValue = np.array([21,9,6])
In [91]: linalg.solve(numArray,numArrValue)
                                                Use solve
Out[91]: array([ 4.95, 4.35, -1.95])
                                                method
```





Finding determinate value

- The determinate value is calculate for the square matrix.
- Determinate value help to find inverse of matrix.
- It represent using |A| where A is my square matrix.
- Determinate calculate on the diagonals value of square matrix.
- For more about determinate :
 https://www.mathsisfun.com/algebra/matrix-determinant.html

For a 2×2 matrix (2 rows and 2 columns):

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

The determinant is:

$$|A| = ad - bc$$

"The determinant of A equals a times d minus b times c"

Image Source: https://www.mathsisfun.com





For a 3×3 matrix (3 rows and 3 columns):

$$\mathbf{A} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

The determinant is:

$$|A| = a(ei - fh) - b(di - fg) + c(dh - eg)$$

"The determinant of A equals ... etc"

It may look complicated, but there is a pattern:

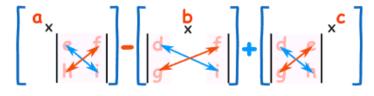


Image Source: https://www.mathsisfun.com





Finding determinate for 2 X 2 matrix

```
In [15]: #for finding determinate linalg.det() function is use
    from scipy import linalg
    import numpy as np
    #Declaring the numpy array
    A = np.array([[5,9],[8,4]])
    print(A)
    #Passing the values to the det function
    x = linalg.det(A)
    #printing the result
    print("determinate of given matrix is :", x)
[[5 9]
    [8 4]]
    determinate of given matrix is : -52.0
```





Finding Determinate for 3 X 3 matrix

```
In [16]: #for finding determinate linalg.det() function is use
    from scipy import linalg
    import numpy as np
    #Declaring the numpy array
    A = np.array([[10,5,8],[8,4,11],[12,4,6]])
    print(A)
    #Passing the values to the det function
    x = linalg.det(A)
    #printing the result
    print("determinate of given matrix is :", x)
[[10 5 8]
    [ 8 4 11]
    [12 4 6]]
    determinate of given matrix is : 92.0
```

Like wise you can find for 4 X 4 for any n X n matrix where n is any integer number





Inverse of matrix

- Inverse of matrix represent with the reciprocal of number. If 8 is one number than reciprocal of 8 is 1/8 and it represent 8^{-1.}
- The Inverse of a Matrix is the same idea but we write it A-1.
- Why inverse of matrix is required? because we can not divide the matrix but when we multiply actual matrix with it inverse matrix than we get

identity matrix.

2x2 Matrix

OK, how do we calculate the inverse?

Well, for a 2x2 matrix the inverse is:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

determinant

Image Source: https://www.mathsisfun.com







Inverse of 2 x 2 matrix

```
In [22]: #inverse of matrix
         from scipy import linalg
         import numpy as np
         #Declaring the numpy array
         A = np.array([[5,9],[8,4]])
         print(A)
         inv mat = linalg.inv(A)
         print("inverse of matrix is : ",inv_mat)
         print("checking the answer, mutiplication should be identity")
         ans = A * inv mat
         ans = ans.astype(int)
         print(ans)
         [[5 9]]
          [8 4]]
         inverse of matrix is : [[-0.07692308  0.17307692]
          [ 0.15384615 -0.09615385]]
         checking the answer, mutiplication should be identity
         [[0 1]
          [1 0]]
```







Inverse of 3 X 3 matrix

```
In [23]: A = np.array([[1,5,9],[8,4,10],[12,4,5]])
         print(A)
         inv_mat = linalg.inv(A)
         print("inverse of matrix is : ",inv_mat)
         print("checking the answer, mutiplication should be identity")
         ans = A * inv mat
         ans = ans.astype(int)
         print(ans)
         [[1 5 9]
          [8 4 10]
          [12 4 5]]
         inverse of matrix is : [[-0.08474576  0.04661017  0.05932203]
          [ 0.33898305 -0.43644068  0.26271186]
          [-0.06779661 0.23728814 -0.15254237]]
         checking the answer, mutiplication should be identity
         [[0 0 0]]
          [2-12]
          [0 0 0]]
```





Singular-Value Decomposition (SVD)

- SVD Is use for matrix decomposition mean reduce the matrix.
- A = U . Sigma . V^T
- Where A is the real m x n matrix that we wants to decompose,
- U is an m x m matrix,
- Sigma (often represented by Greek letter Sigma) is an m x n diagonal matrix, V^T is the transpose of an n x n matrix where T is a superscript.

Image Source : https://www.mathsisfun.com







```
In [25]: from numpy import array
         from scipy.linalg import svd
         # define a matrix
         A = array([[1, 2], [3, 4], [5, 6]])
         # SVD
         U, s, VT = svd(A)
         print("Unitery Matrix")
         print(U)
         print("Sigma / Square root of Eigenvale")
         print(s)
         print("VH value ")
         print(VT)
         Unitery Matrix
         [[-0.2298477 0.88346102 0.40824829]
          [-0.52474482 0.24078249 -0.81649658]
          [-0.81964194 -0.40189603 0.40824829]]
         Sigma / Square root of Eigenvale
         [9.52551809 0.51430058]
         VH value
         [[-0.61962948 -0.78489445]
          [-0.78489445 0.61962948]]
```



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```
In [103]:
           import numpy as np
                                                                              Import linalg
           from scipy import linalg
                                                                              Define matrix
In [104]:
           numSvdArr = np.array([[3,5,1],[9,5,7]])
                                                                             Find shape of ndarray which
In [105]:
           numSvdArr.shape
                                                                             is 2X3 matrix
Out[105]: (2L, 3L)
                                                                             Use syd function
In [106]:
           linalg.svd(numSvdArr)
Out[106]: (array([[-0.37879831, -0.92547925],

    U (Unitary matrix)

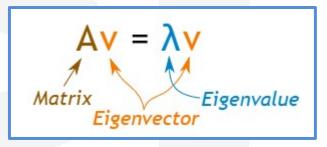
                    [-0.92547925, 0.37879831]]),
                                                                    Sigma or square root of eigenvalues
            array([ 13.38464336, 3.29413449]),
            array([[-0.7072066 , -0.4872291 , -0.51231496],
                    [ 0.19208294, -0.82977932, 0.52399467],
                                                                               VH is values collected into
                    [-0.68041382, 0.27216553, 0.68041382]]))
                                                                               unitary matrix
```





Calculate Eigenvalues and Eigenvector

- Finding Eigenvalue and Eigenvector are the most common problem for any linear algebraic equation.
- It is calculated for square matrix i.e. (2X2, 3X3 or any square matrix)
- Is calculated using :



- Where A is any square matrix
- V is any n X 1 vector for real numbers
- λ is a scalar (which may be either real or complex)
- For more:

https://lpsa.swarthmore.edu/MtrxVibe/EigMat/MatrixEigen.html https://www.mathsisfun.com/algebra/eigenvalue.html







How to find Eigenvalue for the given matrix

Example: Solve for λ :

Start with $| A - \lambda I | = 0$

$$\left| \begin{bmatrix} -6 & 3 \\ 4 & 5 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right| = 0$$

Which is:

$$\begin{vmatrix} -6-\lambda & 3 \\ 4 & 5-\lambda \end{vmatrix} = 0$$

Calculating that determinant gets:

$$(-6-\lambda)(5-\lambda) - 3\times 4 = 0$$

Which then gets us this Quadratic Equation:

$$\lambda^2 + \lambda - 42 = 0$$

And (solving it) gets:

$$\lambda = -7 \text{ or } 6$$

And yes, there are two possible eigenvalues.





Find eigenvector for eigenvalues

Example (continued): Find the Eigenvector for the Eigenvalue $\lambda = 6$:

Start with:

$$Av = \lambda v$$

Put in the values we know:

$$\begin{bmatrix} -6 & 3 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 6 \begin{bmatrix} x \\ y \end{bmatrix}$$

After multiplying we get these two equations:

$$-6x + 3y = 6x$$
$$4x + 5y = 6y$$



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Cont...

Bringing all to left hand side:

$$-12x + 3y = 0$$
$$4x - 1y = 0$$

Either equation reveals that y = 4x, so the eigenvector is any non-zero multiple of this:

 $\begin{bmatrix} 1 \\ 4 \end{bmatrix}$

And we get the solution shown at the top of the page:

$$\begin{bmatrix} -6 & 3 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} 1 \\ 4 \end{bmatrix} = \begin{bmatrix} -6 \times 1 + 3 \times 4 \\ 4 \times 1 + 5 \times 4 \end{bmatrix} = \begin{bmatrix} 6 \\ 24 \end{bmatrix}$$

... and also ...

$$6\begin{bmatrix}1\\4\end{bmatrix} = \begin{bmatrix}6\\24\end{bmatrix}$$

So
$$AV = \lambda V$$





Let's find it using python scipy

```
In [1]: #importing the scipy and numpy packages
    from scipy import linalg
    import numpy as np
    #Declaring the numpy array
    a = np.array([[3,2],[4,6]])
    #Passing the values to the eig function
    l, v = linalg.eig(a)
    #printing the result for eigenvalues
    print(l)
    #printing the result for eigenvectors
    print(v)

[1.29843788+0.j 7.70156212+0.j]
[[-0.76164568 -0.39144501]
    [ 0.64799372 -0.9202015 ]]
```





SciPy Sub Package - Statistics

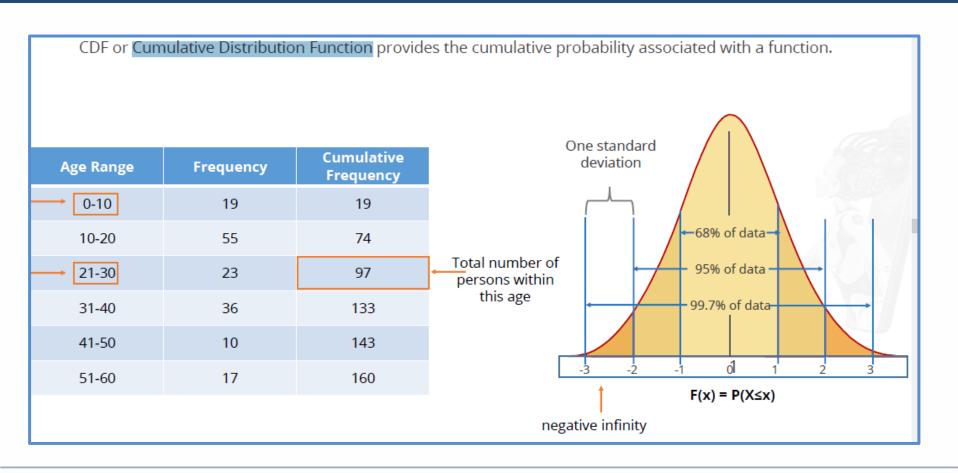
- As for data science and data analytics statistics plays very important role so sicpy have rich set of function to perform calculation based on statistics.
- All the function are located into scipy.stats package.
- A list of random variables available can also be obtained from the docstring for the stats sub-package.
- We can get to know list of function supported by stats package using info(stats).

Function	Description
rv_continuos	It is a base class to construct specific distribution classes and instances for continuous random variable.
rv_discrete	It is a base class to construct specific distribution classes and instances for discrete random variables.
rv_histogram	It can be inherited from rv_continuous class. It generates a distribution given by a histogram.





Normal Continuous Random Variable

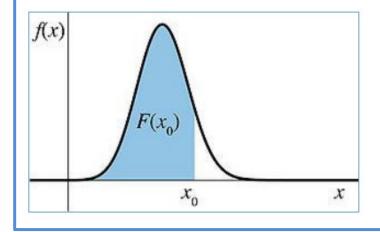








Probability Density Function, or **PDF**, of a continuous random variable is the derivative of its Cumulative Distribution Function, or CDF.



$$f(x) = \frac{dF(x)}{dx}$$
 Derivative of CDF







```
In [1]: # two general distribution classes which have been implemented for encapsulating
        # is continuous random variables and discrete random variable
        # calculating Cumulative Distribution Function
        from scipy.stats import norm
        import numpy as np
        print(norm.cdf(np.array([3,-1., 0, 1, 2, 4, -2, 5])))
        [0.9986501 0.15865525 0.5
                                          0.84134475 0.97724987 0.99996833
         0.02275013 0.99999971]
In [4]: #To get the median of the distribution, we can use the Percent Point Function (PPF),
        #PPF is the inverse of the CDF.
        from scipy.stats import norm
        print(norm.rvs(size = 4))
        #output for rvs is change with every execution
        #for getting fix value use seed() function
        [ 0.55359238 -1.55145107 -0.68957377 -0.0369672 ]
```







Sho	own here are functions used to perform Normal Distribution:
In [108]:	from scipy.stats import norm Import norm distribution
In [110]:	norm.rvs(loc=0,scale=1,size=10) rvs for Random variables
Out[110]:	array([-0.16337774, 0.39039561, 0.85642826, 0.30134358, -1.86009474, -0.29621603, 0.03863757, 0.23727056, -1.42395316, -0.5730162])
In [112]:	norm.cdf(5,loc=1,scale=2) cdf for Cumulative Distribution Function
Out[112]:	0.97724986805182079
In [113]:	norm.pdf(9,loc=0,scale=1) — pdf for Probability Density
Out[113]:	Function for random distribution
	loc and scale are used to adjust the location and scale of the data distribution.





SciPy Sub-Package: Weave and IO

- Scipy have many module, classes and function to read and write operation for file and data from various source.
- But scipy.io package provide wide range of function to for working on file read write operation. It support many file formats like below.
- Idl, Matlab, Matrix Market, Arff, Wave, Netcdf, etc.
- But for now we only concentrate on wave file type.
- For more you can visit :
 https://www.tutorialspoint.com/scipy/scipy input output.htm
- https://www.javatpoint.com/scipy-input-and-output







The weave package provides ways to modify and extend any supported extension libraries.



Features of Weave Package:

- Includes C/C++ code within Python code
- Speed ups of 1.5x to 30x compared to algorithms written in pure Python

Two main functions of weave::

- inline() compiles and executes C/C++ code on the fly
- blitz() compiles NumPy Python expressions for fast execution





example

```
In [1]: import scipy.io as sio
        import numpy as np
        #Save a mat file
        vect = np.arange(10)
        sio.savemat('array.mat', {'vect':vect})
        #Now Load the File
        mat file content = sio.loadmat('array.mat')
        print(mat file content)
        {' header ': b'MATLAB 5.0 MAT-file Platform: nt, Created on: Thu Dec 31 20:56:35 2020', ' version ': '1.0', ' globals ':
        [], 'vect': array([[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]])}
In [2]: #array consisted with the information. If we want to inspect the contents of a MATLAB file without
        #reading the data into memory
        #use the whosmat command
        import scipy.io as sio
        mat_file_content = sio.whosmat('array.mat')
        print(mat file content)
        [('vect', (1, 10), 'int32')]
```





For more about scipy

- https://www.tutorialspoint.com/scipy/index.htm
- https://docs.scipy.org/doc/scipy/reference/tutorial/
- https://www.guru99.com/scipy-tutorial.html#4
- https://scipy-lectures.org/
- https://www.javatpoint.com/scipy-installation
- https://www.journaldev.com/18106/python-scipy-tutorial
- https://www.w3schools.com/python/scipy intro.asp

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