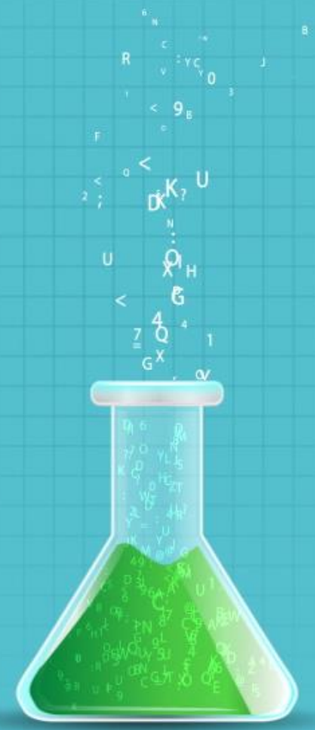
Data Science with Python

Lesson 06—Python: Scientific computing with Python (SciPy)

DATA SCIENCE

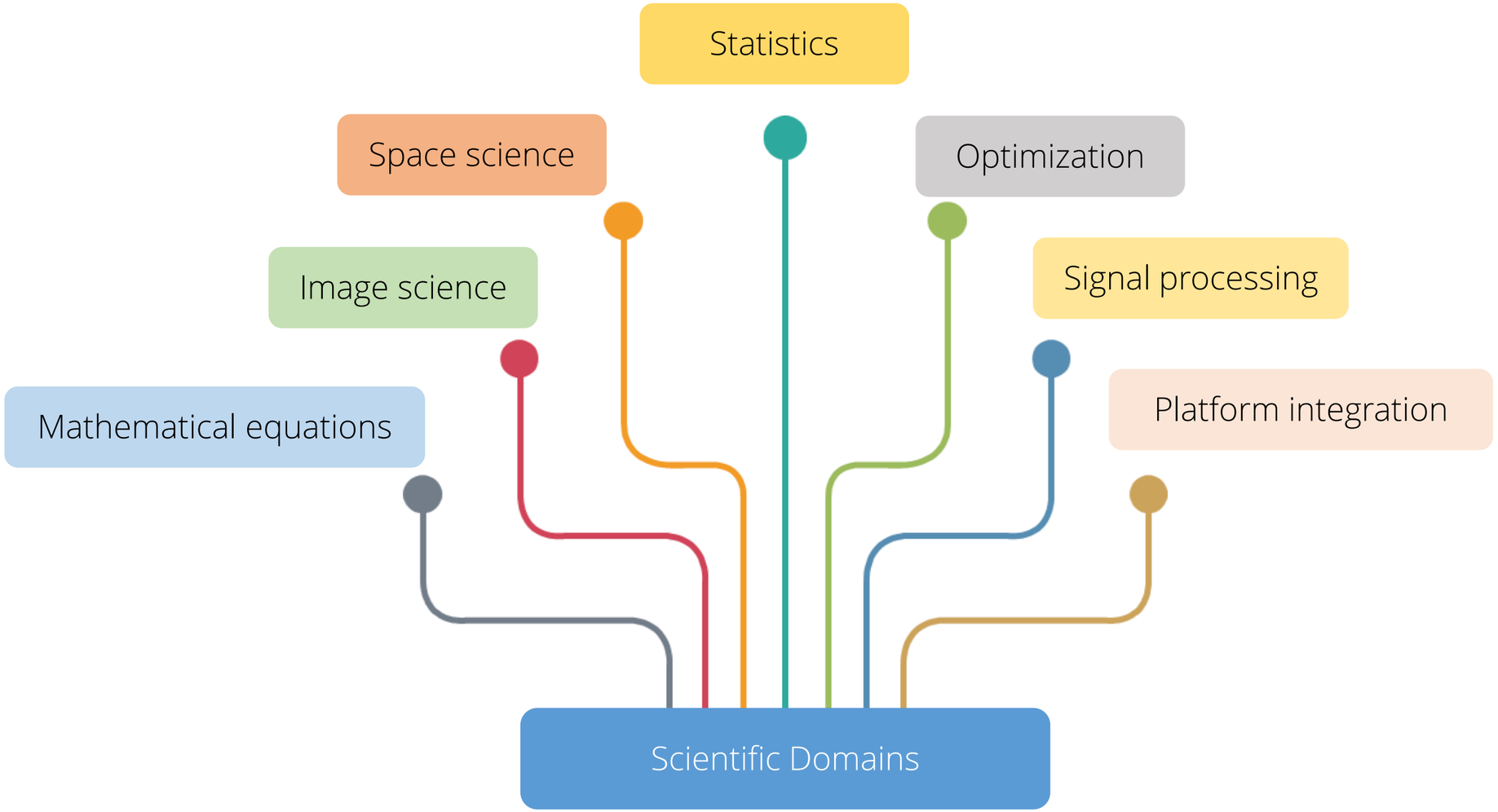
What You'll Learn

- Why SciPy is needed
- The characteristics of SciPy
- The sub-packages of SciPy
- SciPy Sub-packages such as Optimization, Integration, Linear Algebra, Statistics, Weave, and IO



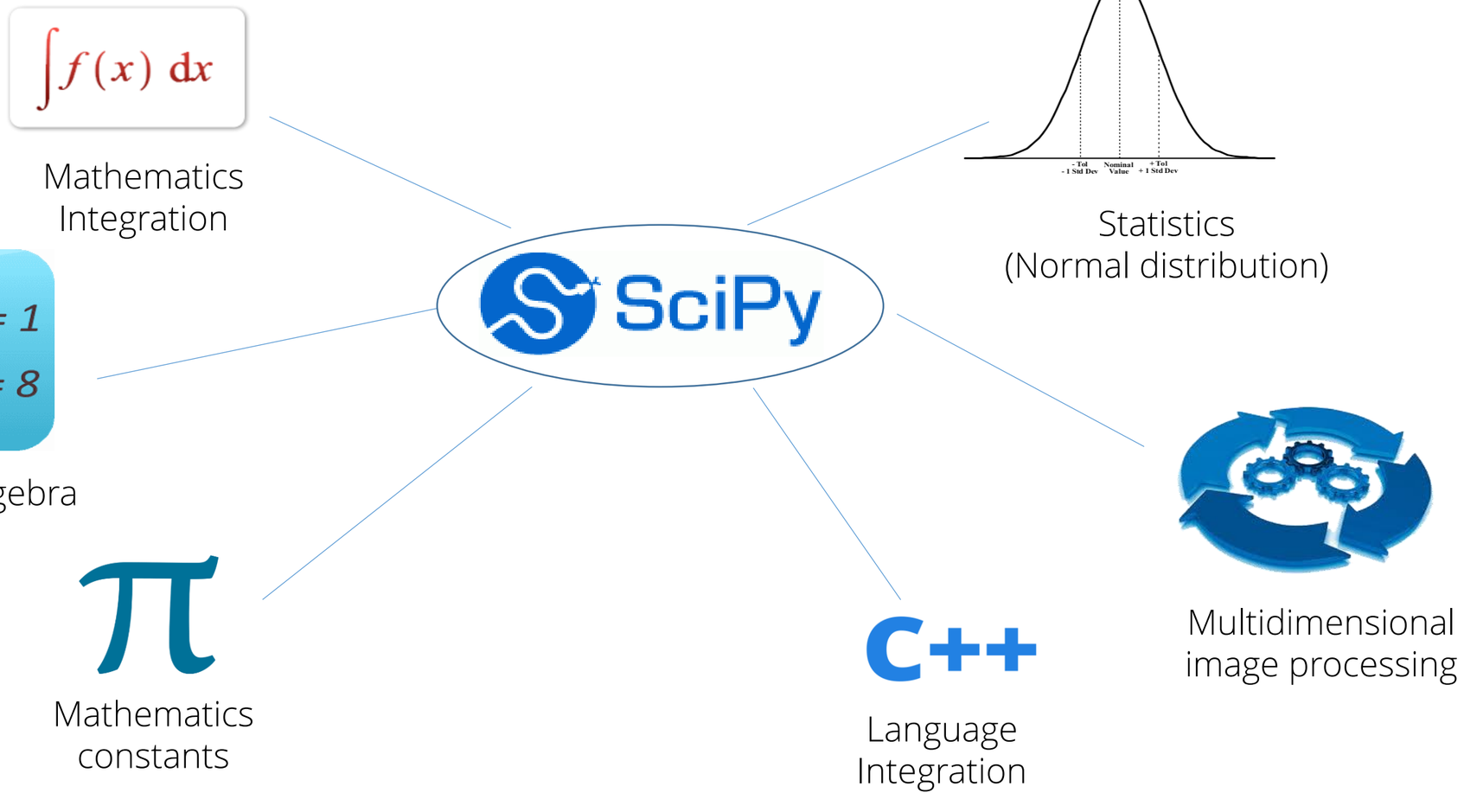
The Real World: Multiple Scientific Domains

How to handle multiple scientific domains? The solution is SciPy.



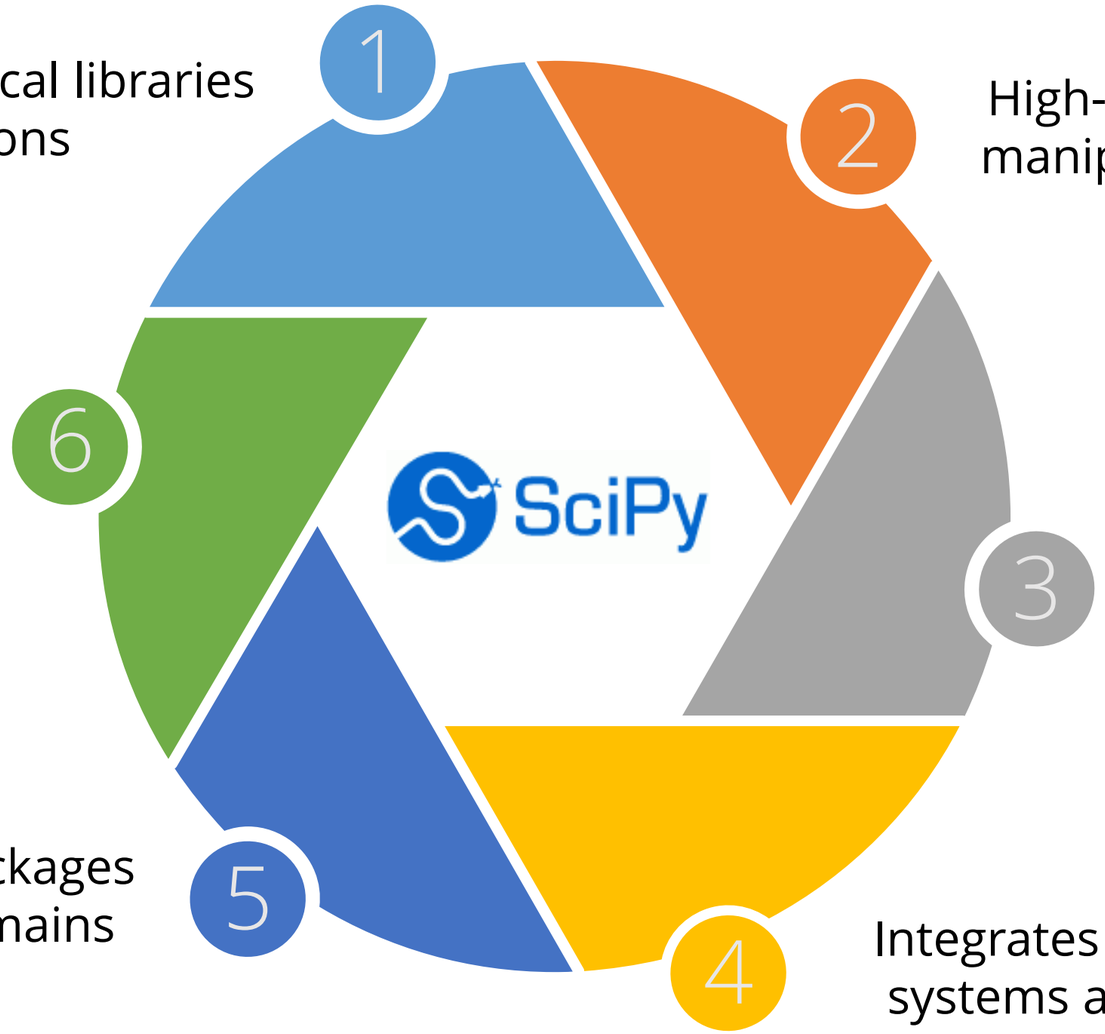
SciPy: The Solution

SciPy has built-in packages that help in handling the scientific domains.



SciPy and its Characteristics

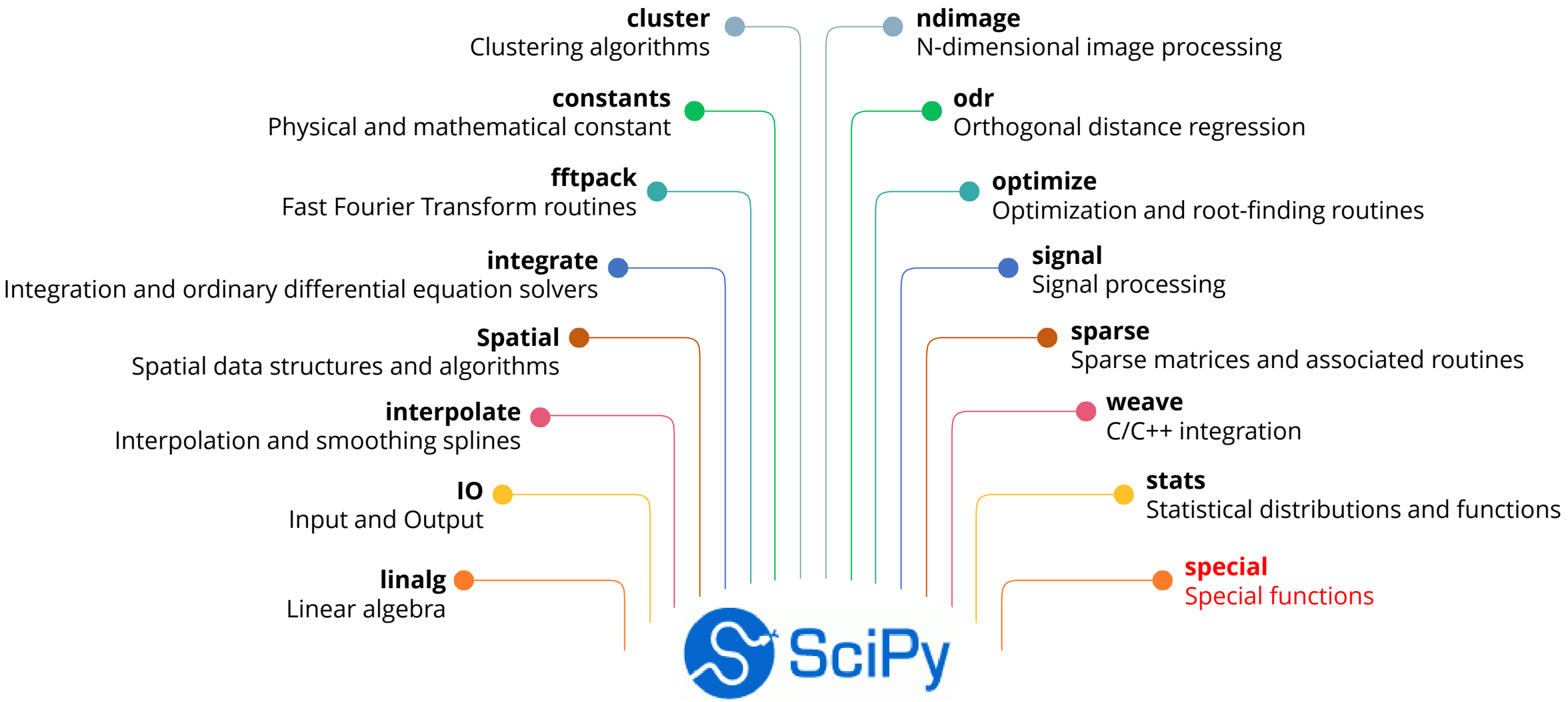
Characteristics of SciPy are as follows:



1. Built-in mathematical libraries and functions
2. High-level commands for data manipulation and visualization
3. Efficient and fast data processing
4. Integrates well with multiple systems and environments
5. Large collection of sub-packages for different scientific domains
6. Simplifies scientific application development

SciPy Sub-package

SciPy has multiple sub-packages which handle different scientific domains.

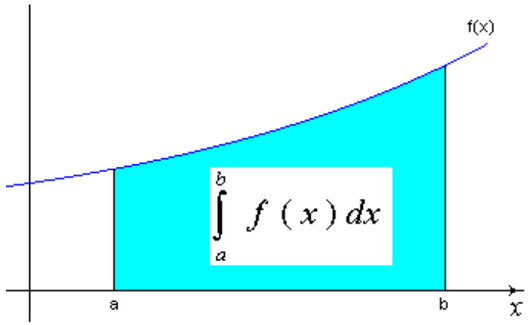


SciPy Sub-package: Integration

SciPy provides integration techniques that solve mathematical sequences and series, or perform function approximation.

General integration (quad)

- integrate.quad(f, a, b)



General multiple integration (dblquad, tplquad, nquad)

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

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

SciPy Sub-package: Integration

This example shows how to perform quad integration.

```
In [13]: from scipy.integrate import quad
```

Import quad from integrate sub-package

```
In [14]: def integrateFunction(x):
             return x
```

Define function for integration of x

```
In [15]: quad(integrateFunction,0,1)
Out[15]: (0.5, 5.551115123125783e-15)
```

Perform quad integration for function of x for limit 0 to 1

```
In [16]: def integrateFn(x,a,b):
             return x*a+b
```

Define function for ax + b

```
In [17]: a=3
         b=2
```

Declare value of a and b

```
In [18]: quad(integrateFn,0,1,args=(a,b))
Out[18]: (3.5, 3.885780586188048e-14)
```

Perform quad integration and pass functions and arguments

SciPy Sub-package: Integration

This example shows you how to perform multiple integration.

```
In [20]: import scipy.integrate as integrate
```

Import integrate package sub-package

```
In [21]: def f(x, y):
             return x + y
         integrate.dblquad(f, 0, 1,lambda x: 0, lambda x: 2)
```

Define function for x + y

```
Out[21]: (3.0, 3.3306690738754696e-14)
```

Perform multiple integration using the lambda built-in function

SciPy Sub-package: Optimization

Optimization is a process to improve performance of a system mathematically by fine-tuning the process parameters.

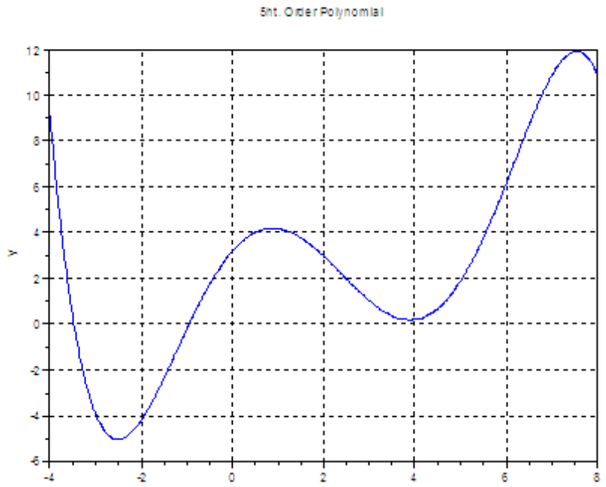
SciPy provides several optimization algorithms such as bfgs, Nelder-Mead simplex, Newton Conjugate Gradient, COBYLA, or SLSQP.

Minimization functions

optimize.minimize(f, x0, method='BFGS')

lower limit in a given range

Root finding, Curve fitting



root(f, x0, method='hybr')

optimize.curve_fit(f, xdata, ydata)

SciPy Sub Package: Optimization

```
In [32]: import numpy as np
         from scipy import optimize
```

Import numpy and optimize from scipy

```
In [33]: def f(x):
             return x**2 + 5*np.sin(x)
```

Define function for X^2 + 5 sin x

```
In [34]: minimaValue = optimize.minimize(f,x0=2,method='bfgs',options={'disp':True})
```

```
Optimization terminated successfully.
         Current function value: -3.246394
         Iterations: 4
         Function evaluations: 24
         Gradient evaluations: 8
```

Perform optimize minimize function using bfgs method and options

```
In [35]: minimaValueWithoutOpt = optimize.minimize(f,x0=2,method='bfgs')
```

```
In [36]: minimaValueWithoutOpt
```

```
Out[36]:       fun: -3.2463942726915382
 hess_inv: array([[ 0.15430551]])
      jac: array([ -8.94069672e-08])
  message: 'Optimization terminated successfully.'
     nfev: 24
      nit: 4
     njev: 8
   status: 0
  success: True
        x: array([-1.11051051])
```

Perform optimize minimize function using bfgs method and without options

SciPy Sub-package: Optimization

```
In [118]: import numpy as np
          from scipy.optimize import root
          def rootfunc(x):
              return x + 3.5 * np.cos(x)
```

Define function for X + 3.5 Cos x

```
In [119]: rootValue = root(rootfunc, 0.3)
```

Pass x value in argument for root

```
In [120]: rootValue
```

```
Out[120]:      fjac: array([[-1.]])
                fun: array([  2.22044605e-16])
            message: 'The solution converged.'
               nfev: 14
                qtf: array([ -8.32889313e-13])
                  r: array([-4.28198145])
             status: 1
            success: True
                  x: array([-1.21597614])
```

Function value and array values

Knowledge Check

KNOWLEDGE CHECK

What are the specification limits provided for curve fitting function (**optimize.curve.fit)**, during the optimization process?

a. Upper limit value

b. Lower limit value

c. Upper and lower limit values

d. Only the optimization method

KNOWLEDGE CHECK

What are the specification limits provided for curve fitting function (**optimize.curve.fit**), during the optimization process?

a. Upper limit value

b. Lower limit value

c. Upper and lower limit values

d. Only the optimization method

The correct answer is c

Explanation: Both the upper and lower limit values should be specified for **optimize.curve.fit** function.

SciPy Sub-package: Linear Algebra

SciPy provides rapid linear algebra capabilities and contains advanced algebraic functions.

Click each tab to know more.

Inverse of matrix	Determinant	Linear systems	Single value decomposition (svd)

This function is used to compute the inverse of the given matrix. Let's take a look at the inverse matrix operation.

```
In [65]: import numpy as np
         from scipy import linalg
         matrix = np.array([[10,6],[2,7]])
         matrix

Out[65]: array([[10,  6],
                [ 2,  7]])

In [66]: type(matrix)

Out[66]: numpy.ndarray

In [67]: linalg.inv(matrix)

Out[67]: array([[ 0.12068966, -0.10344828],
                [-0.03448276,  0.17241379]])
```

Import linalg and Define a numpy matrix or array

View the type

Use inv function to inverse the matrix

SciPy Sub-package: Linear Algebra

SciPy provides very rapid linear algebra capabilities and contains advanced algebraic functions.

Click each tab to know more.

Inverse of matrix	Determinant	Linear systems	Single value decomposition (svd)

With this function you can compute the value of the determinant for the given matrix.

```
In [68]: import numpy as np
         from scipy import linalg
         matrix = np.array([[4,9],[3,5]])
         matrix

Out[68]: array([[4, 9],
                [3, 5]])

In [69]: linalg.det(matrix)

Out[69]: -7.000000000000001
```

Import linalg and
Define an numpy matrix or array

Use det function to find the determinant value of the matrix

SciPy Sub-package: Linear Algebra

SciPy provides very rapid linear algebra capabilities and contains advanced algebraic functions.

Click each tab to know more.

Inverse of matrix | Determinant | **Linear systems** | Single value decomposition (svd)

Linear equations

$$2x + 3y + z = 21$$
$$-x + 5y + 4z = 9$$
$$3x + 2y + 9z = 6$$

```
In [88]: import numpy as np
         from scipy import linalg

In [89]: 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)
Out[91]: array([ 4.95,  4.35, -1.95])
```

Import linalg

Use solve method

SciPy Sub-package: Linear Algebra

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Click each tab to know more.

Inverse of matrix	Determinant	Linear systems	Single value decomposition (svd)

```
In [103]: import numpy as np
          from scipy import linalg
```

Import linalg

```
In [104]: numSvdArr = np.array([[3,5,1],[9,5,7]])
```

Define matrix

```
In [105]: numSvdArr.shape
Out[105]: (2L, 3L)
```

Find shape of ndarray which is 2X3 matrix

```
In [106]: linalg.svd(numSvdArr)
Out[106]: (array([[-0.37879831, -0.92547925],
                  [-0.92547925,  0.37879831]]),
           array([ 13.38464336,   3.29413449]),
           array([[-0.7072066 , -0.4872291 , -0.51231496],
                  [ 0.19208294, -0.82977932,  0.52399467],
                  [-0.68041382,  0.27216553,  0.68041382]]))
```

Use svd function

U (Unitary matrix)

Sigma or square root of eigenvalues

VH is values collected into unitary matrix

Demo—Calculate Eigenvalues

Demonstrate how to calculate eigenvalues.

DATA SCIENCE

Knowledge Check

KNOWLEDGE CHECK

Which of the following function is used for inversing the matrix?

a. SciPy.special

b. SciPy.linalg

c. SciPy.signal

d. SciPy.stats

KNOWLEDGE CHECK

Which of the following function is used for inversing the matrix?

a. SciPy.special

b. SciPy.linalg

c. SciPy.signal

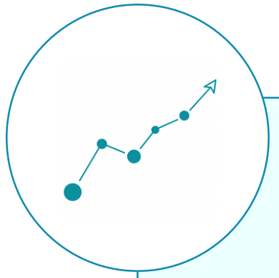
d. SciPy.stats

The correct answer is b

Explanation: SciPy.linalg is used to inverse the matrix.

SciPy Sub-package: Statistics

SciPy provides a very rich set of statistical functions which are as follows:



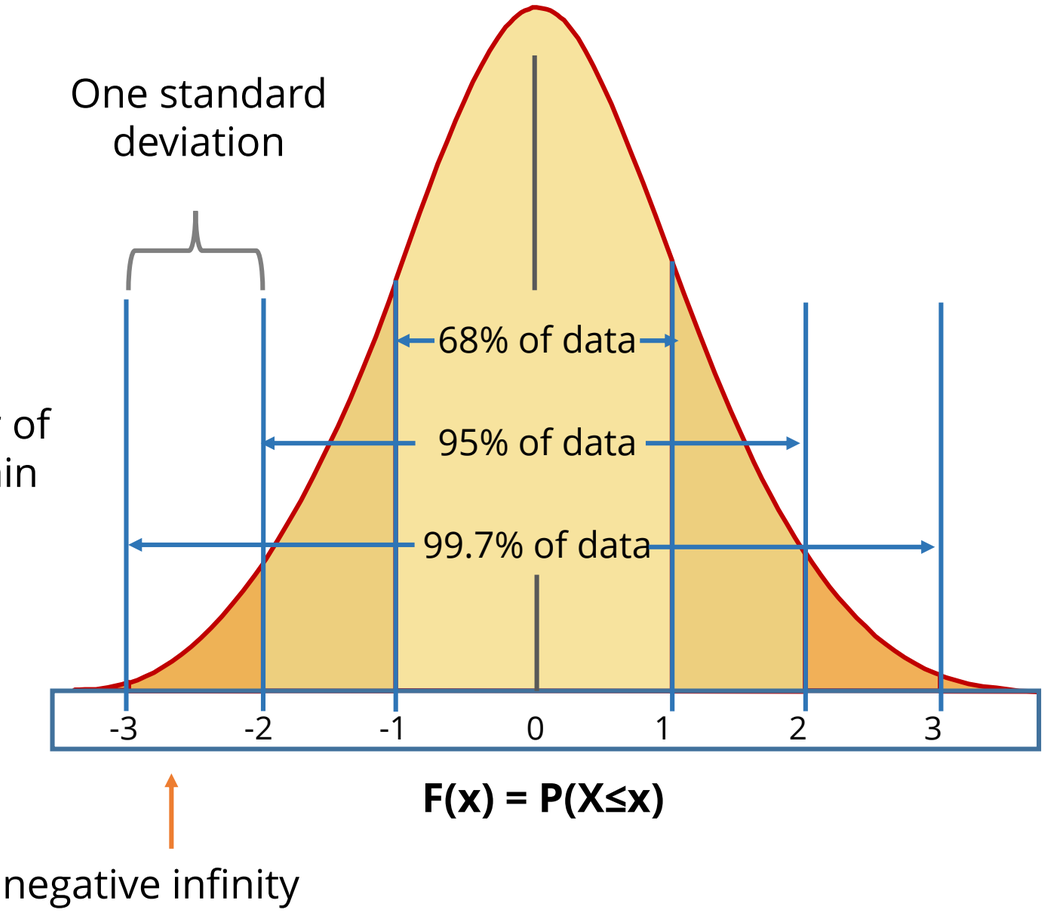
- This package contains distributions for which random variables are generated.
- These packages enable the addition of new routines and distributions. It also offers convenience methods such as pdf(), cdf()
- Following are the statistical functions for a set of data:
  - linear regression: linregress()
  - describing data: describe(), normaltest()

SciPy Sub-package: Statistics

Cumulative Distribution Function provides the cumulative probability associated with a function.

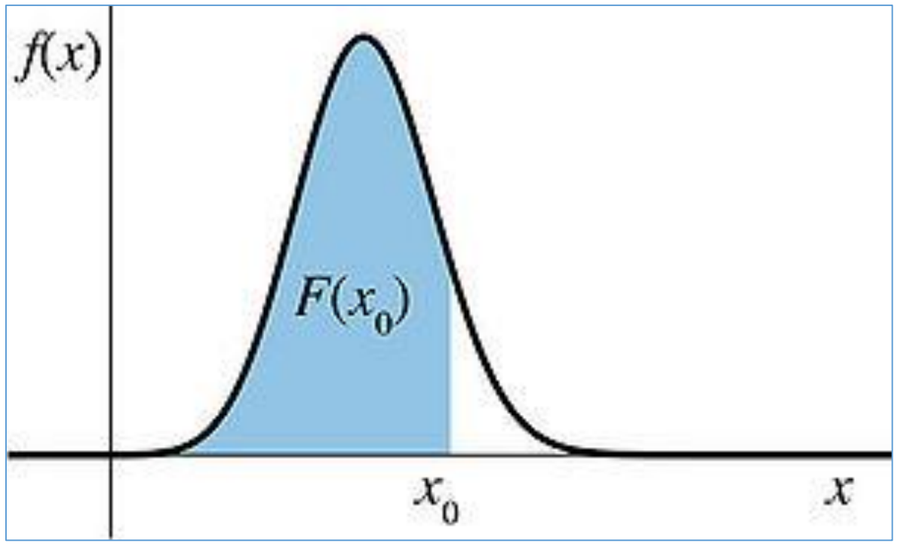
Age Range	Frequency	Cumulative Frequency
0-10	19	19
10-20	55	74
21-30	23	97
31-40	36	133
41-50	10	143
51-60	17	160

Total number of persons within this age



SciPy Sub-package: Statistics

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

SciPy Sub-package: Statistics

Functions of Random Variables – Continuous (Normal Distribution):

```
In [108]: from scipy.stats import norm
```

Import norm for normal distribution

```
In [110]: norm.rvs(loc=0,scale=1,size=10)

Out[110]: array([-0.16337774,  0.39039561,  0.85642826,  0.30134358, -1.86009474,
                 -0.29621603,  0.03863757,  0.23727056, -1.42395316, -0.5730162 ])
```

rvs for Random variables

```
In [112]: norm.cdf(5,loc=1,scale=2)

Out[112]: 0.9772498680518207
```

cdf for Cumulative Distribution Function

```
In [113]: norm.pdf(9,loc=0,scale=1)

Out[113]: 1.0279773571668917e-18
```

pdf for Probability Density Function for random distribution

loc and scale are used to adjust the location and scale of the data distribution.

SciPy Sub-package: Weave

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

- 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

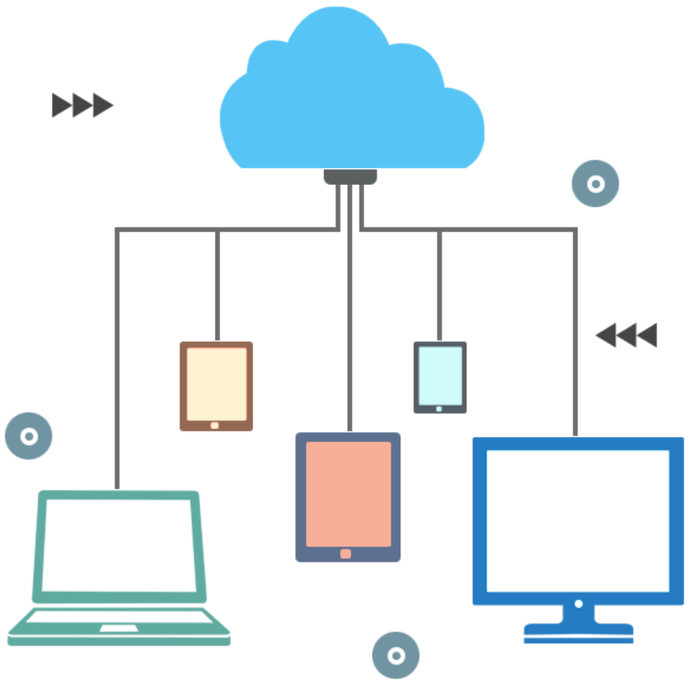
SciPy Sub-package: IO

The IO package provides a set of functions to deal with several kinds of file formats.

It offers a set of functions to deal with file formats that includes:

- MatLab file
- IDL files
- Matrix Market files
- Wav sound files
- Arff files, and
- Netcdf files

Package provides additional files and it’s corresponding methods.



Assignment

Assignment 01

Problem | Instructions

Use SciPy to solve a linear algebra problem.

There is a test with 30 questions worth 150 marks. The test has two types of questions:

1. True or false – carries 4 marks each

2. Multiple choice – carries 9 marks each

Find the number of true or false and multiple choice questions.

Assignment 01

Problem | Instructions

Common instructions:

- If you are new to Python, download the “Anaconda Installation Instructions” document from the “Resources” tab to view the steps for installing Anaconda and the Jupyter notebook.
- Download the “Assignment 01” notebook and upload it on the Jupyter notebook to access it.
- Follow the cues provided to complete the assignment.

Assignment

Assignment 02

Problem | Instructions

Use SciPy to declare 20 random values for random values and perform the following:

1. CDF – Cumulative Distribution Function for 10 random variables.
2. PDF – Probability Density Function for 14 random variables.

Assignment 02

Problem | Instructions

Common instructions:

- If you are new to Python, download the “Anaconda Installation Instructions” document from the “Resources” tab to view the steps for installing Anaconda and the Jupyter notebook.
- Download the “Assignment 02” notebook and upload it on the Jupyter notebook to access it.
- Follow the cues provided to complete the assignment.

Quiz

QUIZ 1

Which of the following is performed using SciPy?

a. Website

b. Plot data

c. Scientific calculations

d. System administration

QUIZ 1

Which of the following is performed using SciPy?

a. Website

b. Plot data

c. Scientific calculations

d. System administration

The correct answer is c.

Explanation: SciPy has been specially made to perform scientific calculations. Generally, Python is the programming language that has libraries to perform all listed activities.

QUIZ 2

Which of the following functions is used to calculate minima?

a. optimize.minimize()

b. integrate.quad()

c. stats.linregress()

d. linalg.solve()

QUIZ 2

Which of the following functions is used to calculate minima?

a. optimize.minimize()

b. integrate.quad()

c. stats.linregress()

d. linalg.solve()

The correct answer is a.

Explanation: The function optimize.minimize() is used to calculate minima. integrate.quad() is used for integral calculation, stats.linregress() is used for linear regression, and linalg.solve() is used to solve a linear system.

QUIZ 3

Which of the following syntaxes is used to generate 100 random variables from a t-distribution with df = 10?

a. stats.t.pmf(df=10, size=100)

b. stats.t.pdf(df=10, size=100)

c. stats.t.rvs(df=10, size=100)

d. stats.t.rand(df=10, size=100)

QUIZ 3

Which of the following syntaxes is used to generate 100 random variables from a t-distribution with df = 10?

a. stats.t.pmf(df=10, size=100)

b. stats.t.pdf(df=10, size=100)

c. stats.t.rvs(df=10, size=100)

d. stats.t.rand(df=10, size=100)

The correct answer is c.

Explanation: The stats.t.rvs() function is used to generate random variables. stats.t.pmf() function is used to generate the probability of mass function, and stats.t.pdf() is used to generate probability density function. Note that stats.t.rand () does not exist.

QUIZ 4

Which of the following functions is used to run C or C++ codes in SciPy?

a. io.loadmat()

b. weave.inline()

c. weave.blitz()

d. io.whosmat()

QUIZ 4

Which of the following functions is used to run C or C++ codes in SciPy?

a. io.loadmat()

b. weave.inline()

c. weave.blitz()

d. io.whosmat()

The correct answer is b.

Explanation: inline() function accepts C codes as string and compiles them for later use. loadmat() loads variables from .mat file. whosmat() checks the variables inside a .mat file.blitz() and then compiles NumPy expressions for faster running, but it can't accept C codes.

Key Takeaways

- SciPy has multiple sub-packages, which proves useful for different scientific computing domains.
- Integration can be used to solve mathematical sequences and series or perform function approximation.
- Optimization is the process to improve performance of a system mathematically by fine-tuning the process parameters.
- The SciPy linear algebraic functions include computing the inverse of a matrix, calculating the determinant, solving linear systems, and computing single value decomposition.
- Statistical functions provide many useful sub-packages that enable the building of a hypothesis, determining the probability, and predicting the outcome.
- The IO package offers a set of functions to deal with several types of file formats.

This concludes “Scientific computing with Python”

The next lesson is “Data Manipulation with Pandas”