

# Scientific Programming

## Lecture A08 – Numpy

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2025/05/28

Acknowledgments: Alberto Montresor, Stefano Teso, Numpy  
Documentation

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# What is Numpy?

Numpy is a freely available library for performing efficient numerical computations over scalars, vectors, matrices, and more generally N-dimensional tensors.

## Features

- Flexible indexing and manipulation of arbitrary dimensional data.
- Many numerical routines (linear algebra, Fourier analysis, local and global optimization, etc.) using a variety of algorithms.
- Clean Python interface to many underlying libraries, which are used as efficient implementations of numerical algorithms.
- Support for random sampling from a variety of distributions.

## Some links

Official Numpy website

`http://www.numpy.org/`

Official documentation

`https://docs.scipy.org/doc/numpy/`

Source code

`https://github.com/numpy/numpy`

## Importing numpy

The customary idiom to import numpy is:

```
import numpy as np
```

Importing specific sub-modules also makes sense, so feel free to write (in this case for the linear algebra module):

```
import numpy.linalg as la
```

# The array class ndarray

An ndarray is an **n-dimensional array** (a.k.a. **tensor**)

- Concepts encountered in analysis and algebra can be implemented as arrays: vectors are 1D arrays, matrices are 2D arrays.
- Given an array, its dimensionality and type can be ascertained by using the **shape**, **ndim** and **dtype** attributes:

```
import numpy as np
x = np.zeros(10)
print(x)           [ 0.  0.  0.  0.  0.  0.  0.  0.  0.  0.]
print(x.shape)    (10,)
print(x.ndim)     1
print(x.dtype)    float64
```

## Creating arrays with various shapes

Creating arrays from scratch can be useful to start off your mathematical code or for debugging purposes.

- Creating an all-zero array with `np.zeros()`
- Creating an all-one array with `np.ones()`

```
import numpy as np
print( np.zeros(2) )           [ 0.  0.]

print( np.ones( (2,2) ) )     [[ 1.  1.]
                               [ 1.  1.]]

print( np.zeros( (2,2,2) ) )  [[[ 0.  0.]
                               [ 0.  0.]]

                               [[ 0.  0.]
                               [ 0.  0.]]]]
```

## Creating arrays with various shapes

To create a diagonal matrix, use the `diag()` and `ones()` methods together.

```
import numpy as np
print( np.diag( np.ones(3) ) )
```

```
[[ 1.  0.  0.]
 [ 0.  1.  0.]
 [ 0.  0.  1.]]
```

## Creating arrays with various shapes

The numpy (more powerful) analogue of `range()` is `np.arange()`.

```
import numpy as np
print( np.arange(10,100,10) )
print( np.arange(0.0,1.0,0.1))
print( np.linspace(0.0,1.0,11))
print( np.diag( np.arange(5) ) )
```

```
10 20 30 40 50 60 70 80 90]
[ 0.  0.1  0.2  0.3  0.4  0.5  0.6  0.7  0.8  0.9]
[ 0.  0.1  0.2  0.3  0.4  0.5  0.6  0.7  0.8  0.9  1. ]
[[0 0 0 0 0]
 [0 1 0 0 0]
 [0 0 2 0 0]
 [0 0 0 3 0]
 [0 0 0 0 4]]
```

## Creating random arrays

- 5-element vector from a uniform distribution in  $[0, \dots, 10[$
- 5-element vector from a normal distribution with  $\mu = 1$  and  $\sigma = 0.2$
- A 3x3 matrix from a uniform distribution over  $\{0, 1\}$

```
import numpy as np
print(np.random.uniform(0, 10, size=5))
print(np.random.normal(1, 0.2, size=5))
print(np.random.randint(0, 2, size=(3, 3)))
```

[ 7.91700684 7.41652128 8.1393401 0.8123227 5.50427964]

[ 1.14191823 0.89203955 1.09505607 0.8081311 0.82282836]

[[0 0 0]  
 [0 1 1]  
 [0 1 1]]

# Creating random arrays

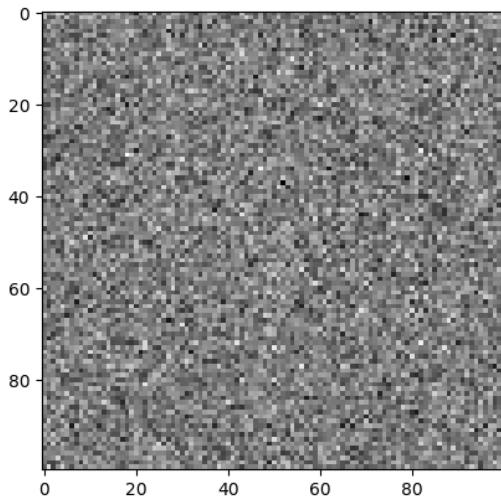
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(0)

rm = np.random.normal(0, 1, size=(100, 100))

plt.imshow(rm, cmap="gray", interpolation="nearest")
plt.savefig("random-matrix.png")
```

# Creating random arrays



## From pandas to numpy and back

It is very easy to “convert” a `Series` or `DataFrame` into an array: as a matter of facts, these Pandas types are built on numpy arrays: their underlying array is accessible through the `values` attribute.

```
import pandas as pd
import numpy as np
iris = pd.read_csv("iris.csv")
print(type(iris.PetalWidth.values))
```

```
<type 'numpy.ndarray'>
```

## Re-shaping, un-raveling

The arrangement of entries into rows, columns, tubes, etc. can be changed at any time using the `reshape()` and `ravel()` methods:

- `reshape()` reshapes an array
- `ravel()` flattens an array into a vector

```
import numpy as np
x = np.arange(9)
print(x)                    [0 1 2 3 4 5 6 7 8]
y = x.reshape((3, 3))
print(y)                    [[0 1 2]
                           [3 4 5]
                           [6 7 8]]
z = y.ravel()
print(z)                    [0 1 2 3 4 5 6 7 8]
```

## Iterating over an array

It is possible to iterate over arrays in several ways:

- Iteration over all elements of an `ndarray`

```
for element in A.flat:  
    print(element)
```

- Iteration over multidimensional arrays is done on slices in the first dimension

```
for row in A:  
    print(row)
```

# Indexing

- `x[i,j]` extracts the element in row `i`, column `j` – just like in standard matrix algebra.
- You can also use the colon `:` notation to select specify all the elements on an axis (e.g. a column, a row, a sub-array).

```
import numpy as np
x = np.arange(9).reshape((3, 3))
print(x)
print(x[0,:]) # First row
print(x[:,0]) # First column
print(x[1:3, :]) # Subarray
```

```
[[0 1 2]
 [3 4 5]
 [6 7 8]]
[0 1 2]
[0 3 6]
[[3 4 5]
 [6 7 8]]
```

# Indexing

The same syntax applies to the n-dimensional case

```
import numpy as np
x = np.arange(5*5).reshape((5,)*5)
print(x.shape)
print(x[0,0,:,:,:])
```

```
(5, 5, 5, 5, 5)
[[ 0  5 10 15 20]
 [25 30 35 40 45]
 [50 55 60 65 70]
 [75 80 85 90 95]
 [100 105 110 115 120]]
```

## Multi-dimensional arrays

It can be difficult to conceptualize operations over  $n$ -dimensional arrays, when  $n$  is larger than 3, unless they have concrete semantics.

### Example

Assume that a 4D array holds the performance of several sequence alignment algorithms over multiple sequence clusters in multiple DBs:

- The first axis is the index of the algorithm
- The second axis is the index of the database
- The third axis is the index of a cluster of sequences
- The fourth axis is one of three measures of performance: precision, recall, and accuracy

## Multi-dimensional arrays

Your tensor looks like this:

```
performances[alg][db][cluster][measure]
```

You may define symbolic constants to identify the indexes of the columns. E.g.,

```
NEEDLEMAN = 0 # Needleman-Wunsch
```

```
SMITH = 1     # Smith-Waterman
```

```
PRECISION = 0
```

```
RECALL = 1
```

```
ACCURACY = 2
```

To extract the accuracy of the Needleman-Wunsch algorithm over all databases and sequence clusters, you can just do:

```
print(performances[NEEDLEMAN, :, :, ACCURACY])
```

# Arithmetic broadcasting

Operations between scalars and arrays are broadcast, like in Pandas (and more generally in linear algebra)

```
import numpy as np
x = np.arange(5)*10
print(x)           [ 0 10 20 30 40]
y = -x
print(y)          [  0 -10 -20 -30 -40]
z = x+y
print(z)          [0 0 0 0 0]
```

# Arithmetic broadcasting

Operations can update the sub-arrays automatically.

```
import numpy as np
x = np.arange(16).reshape((4, 4))
print(x)
x[1:3,1:3] += 100
print(x)
```

```
[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]
 [12 13 14 15]]
```

```
[[ 0  1  2  3]
 [ 4 105 106  7]
 [ 8 109 110 11]
 [ 12 13 14 15]]
```

## Compatible sizes

Operations between arrays of different shapes but compatible sizes are broadcast by “matching” the last (right-most) dimension. e.g, addition between a matrix  $x$  and a vector  $y$  broadcasts  $y$  over all rows of  $x$ :

```
import numpy as np
x = np.arange(9).reshape((3, 3))
print(x)
y = np.arange(3)
print(y)
z = x + y
print(z)
```

```
[[ 0  1  2]
 [ 3  4  5]
 [ 6  7  8]]

[0 1 2]

[[ 0  2  4]
 [ 3  5  7]
 [ 6  8 10]]
```

## Incompatible sizes

Operations between arrays of incompatible sizes raise an error.

```
>>> np.arange(3) + np.arange(2)
```

```
Traceback (most recent call last):
```

```
  File "<stdin>", line 1, in <module>
```

```
ValueError: operands could not be broadcast together with  
shapes (3,) (2,)
```

# Mathematical functions

Numpy contains several mathematical functions, that can be applied to tensors (besides being applicable to scalar values).

<https://docs.scipy.org/doc/numpy/reference/routines.math.html>

## Trigonometric functions

<code>sin</code> (x, /, out, where, casting, order, ...)	Trigonometric sine, element-wise.
<code>cos</code> (x, /, out, where, casting, order, ...)	Cosine element-wise.
<code>tan</code> (x, /, out, where, casting, order, ...)	Compute tangent element-wise.
<code>arcsin</code> (x, /, out, where, casting, order, ...)	Inverse sine, element-wise.
<code>arccos</code> (x, /, out, where, casting, order, ...)	Trigonometric inverse cosine, element-wise.
<code>arctan</code> (x, /, out, where, casting, order, ...)	Trigonometric inverse tangent, element-wise.
<code>hypot</code> (x1, x2, /, out, where, casting, ...)	Given the "legs" of a right triangle, return its hypotenuse.
<code>arctan2</code> (x1, x2, /, out, where, casting, ...)	Element-wise arc tangent of <code>x1/x2</code> choosing the quadrant correctly.
<code>degrees</code> (x, /, out, where, casting, order, ...)	Convert angles from radians to degrees.
<code>radians</code> (x, /, out, where, casting, order, ...)	Convert angles from degrees to radians.
<code>unwrap</code> (p[, discont, axis])	Unwrap by changing deltas between values to $2\pi$ complement.
<code>deg2rad</code> (x, /, out, where, casting, order, ...)	Convert angles from degrees to radians.
<code>rad2deg</code> (x, /, out, where, casting, order, ...)	Convert angles from radians to degrees.

# Mathematical functions

```
import numpy as np
import matplotlib.pyplot as plt

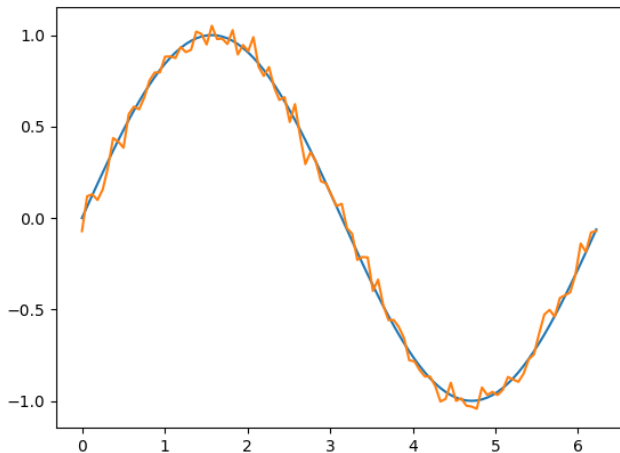
# The x values
x = 2 * np.pi / 100 * np.arange(100)

# The y values, uncorrupted
y = np.sin(x)
plt.plot(x, y)

# The y values, now corrupted by Gaussian noise
y += np.random.normal(0, 0.05, size=100)
plt.plot(x, y)

plt.savefig("sin.png")
```

# Mathematical functions



# Linear Algebra

Numpy provides a number of linear algebraic functions, including dot products, matrix-vector multiplication, and matrix-matrix multiplication.

```
# dot product between vectors
```

```
x = np.array([0, 0, 1, 1])
```

```
y = np.array([1, 1, 0, 0])
```

```
print(np.dot(x, x))
```

```
2
```

```
print(np.dot(y, y))
```

```
2
```

```
print(np.dot(x, y))
```

```
0
```

```
# Matrix-vector product
```

```
a = 2 * np.diag(np.ones(4))
```

```
print(np.dot(a, x))
```

```
[ 0.  0.  2.  2.]
```

```
print(np.dot(a, y))
```

```
[ 2.  2.  0.  0.]
```

```
# Matrix-matrix product
```

```
b = np.ones((4, 4)) - a
```

```
print(np.dot(a, b))
```

```
[[-2.  2.  2.  2.]
```

```
[ 2. -2.  2.  2.]
```

```
[ 2.  2. -2.  2.]
```

```
[ 2.  2.  2. -2.]]
```

# Linear Algebra

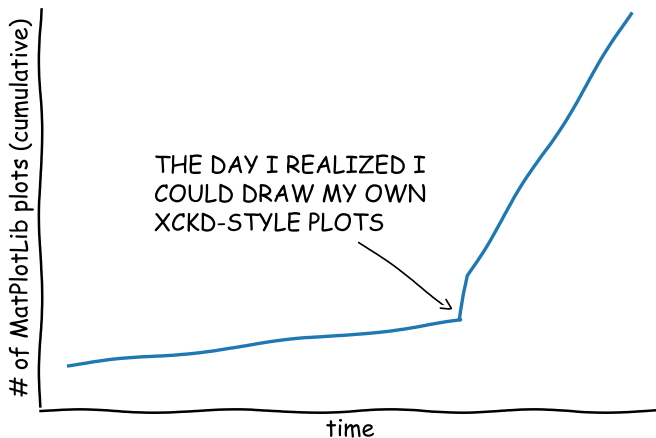
Numpy also provides routines for dealing with eigenvalues/eigenvecs, singular value decompositions, and other decompositions.

```
import numpy as np
import numpy.linalg as la
eigenvalues, eigenvectors =
    la.eig(np.ones((4, 4)))
print(eigenvalues)
print(eigenvectors)
```

```
[ 0.00000000e+00  4.00000000e+00  0.00000000e+00  2.80731443e-32]

[[-0.8660254  -0.5          -0.8660254  -0.64641535]
 [ 0.28867513 -0.5          0.28867513 -0.32788993]
 [ 0.28867513 -0.5          0.28867513  0.48715264]
 [ 0.28867513 -0.5          0.28867513  0.48715264]]
```

# Why use Matplotlib?



# What is Matplotlib?

Matplotlib is a plotting library for the Python programming language and its numerical mathematics extension NumPy

## Two approaches

- The underlying general purpose Matplotlib provides the general framework for plotting several types of figures
- The Matplotlib module `pyplot` provides a declarative way of plotting data, really similar to the syntax of MatLab

`pyplot` is simpler than the general framework, and allows you to produce figures very quickly.

However, the full power is given by the entire framework.

# Matplotlib plotting script

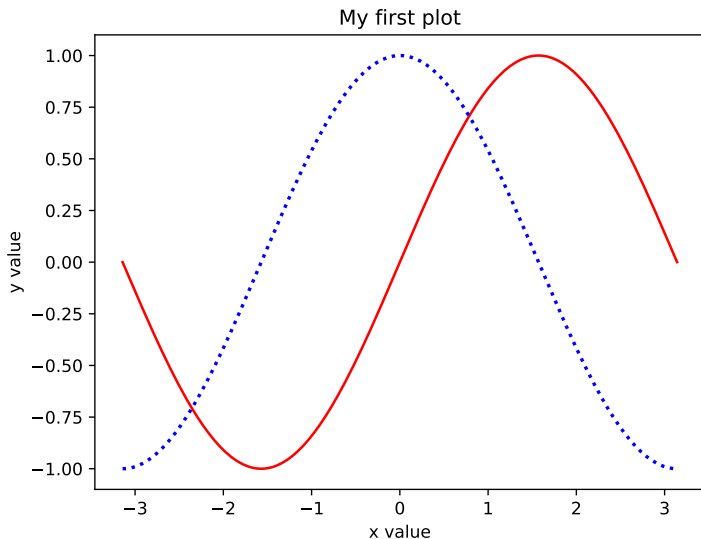
## General structure

- import the required modules  
(`numpy as np` and `matplotlib.pyplot as plt`),
- load or generate some data,
- (optional) customize the appearance of your figure,
- generate a figure (`plot()`, `bar()`, `pie()` etc),
- display it or save it in a file (many formats: PNG, PDF, SVG etc)

## Example 1

```
import numpy as np
import matplotlib.pyplot as plt
x = np.linspace(-np.pi, np.pi, 200)
y1 = np.sin(x)
y2 = np.cos(x)
plt.title("My first plot")
plt.plot(x, y1, "r-")
plt.plot(x, y2, color="blue", linewidth=2.0, linestyle=":")
plt.ylabel('y value')
plt.xlabel('x value')
plt.savefig("figure1.pdf", bbox_inches='tight')
```

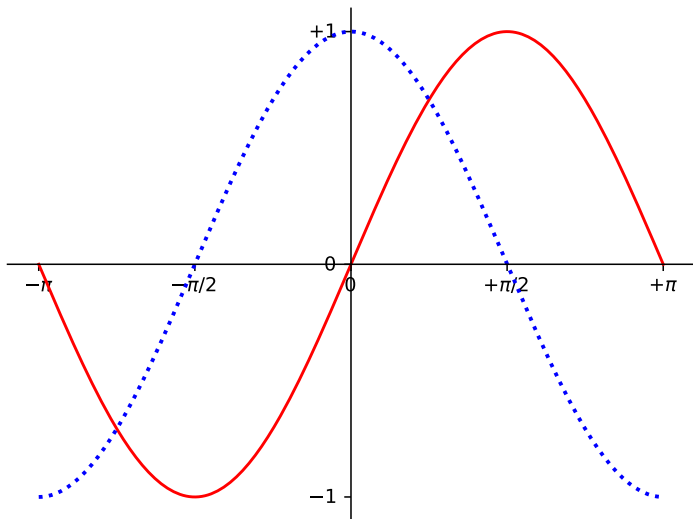
# Example 1



## Example 2

```
plt.xticks([-np.pi, -np.pi/2, 0, np.pi/2, np.pi],
           [r'$-\pi$', r'$-\pi/2$', r'$0$', r'$+\pi/2$', r'$+\pi$'])
plt.yticks([-1, 0, +1],
           [r'$-1$', r'$0$', r'$+1$'])
plt.plot(x, y1, "r-")
plt.plot(x, y2, color="blue", linewidth=2.0, linestyle=":")
ax = plt.gca()
ax.spines['right'].set_color('none')
ax.spines['top'].set_color('none')
ax.xaxis.set_ticks_position('bottom')
ax.spines['bottom'].set_position(('data',0))
ax.yaxis.set_ticks_position('left')
ax.spines['left'].set_position(('data',0))
```

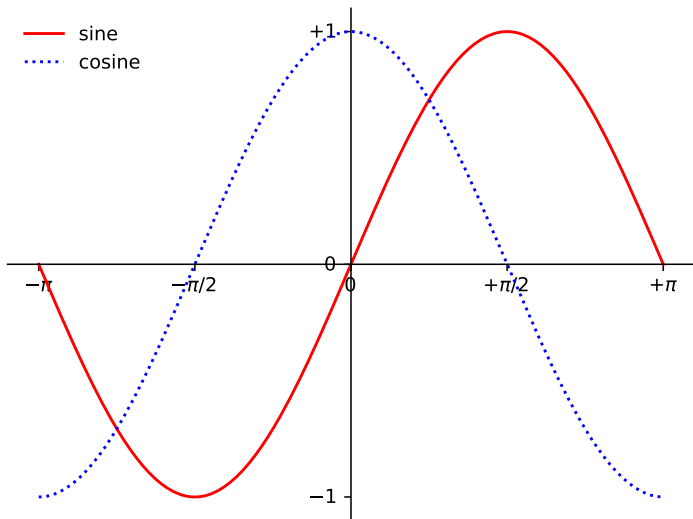
## Example 2



## Example 3

```
plt.plot(x, y1, "r-", label="sine")
plt.plot(x, y2, "b:", label="cosine")
plt.legend(loc='upper left', frameon=False)
```

## Example 3



## Example 4

```

t = 2*np.pi/3
plt.plot([t,t],[0,np.cos(t)], "b--")
plt.scatter([t,],[np.cos(t),], 50, color = 'blue')

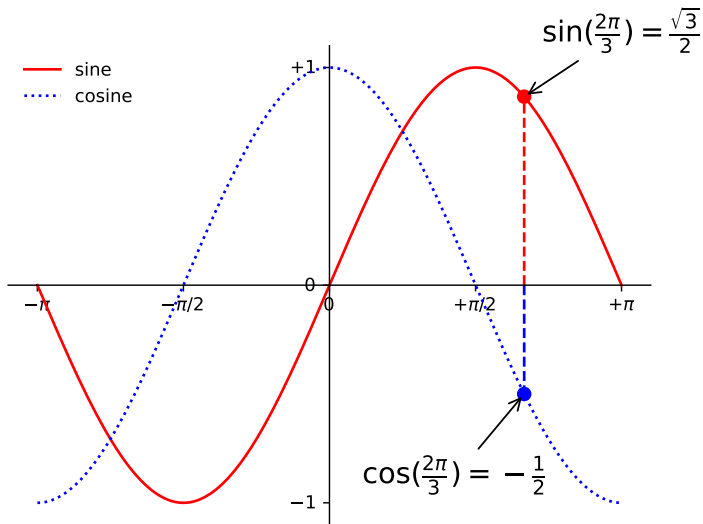
plt.annotate(r'$\sin(\frac{2\pi}{3})=\frac{\sqrt{3}}{2}$',
             xy=(t, np.sin(t)), xycoords='data',
             xytext=(+10, +30), textcoords='offset points',
             fontsize=16, arrowprops=dict(arrowstyle="->"))

plt.plot([t,t],[0,np.sin(t)], "r--")
plt.scatter([t,],[np.sin(t),], 50, color = 'red')

plt.annotate(r'$\cos(\frac{2\pi}{3})=-\frac{1}{2}$',
             xy=(t, np.cos(t)), xycoords='data',
             xytext=(-90, -50), textcoords='offset points',
             fontsize=16, arrowprops=dict(arrowstyle="->"))

```

## Example 4



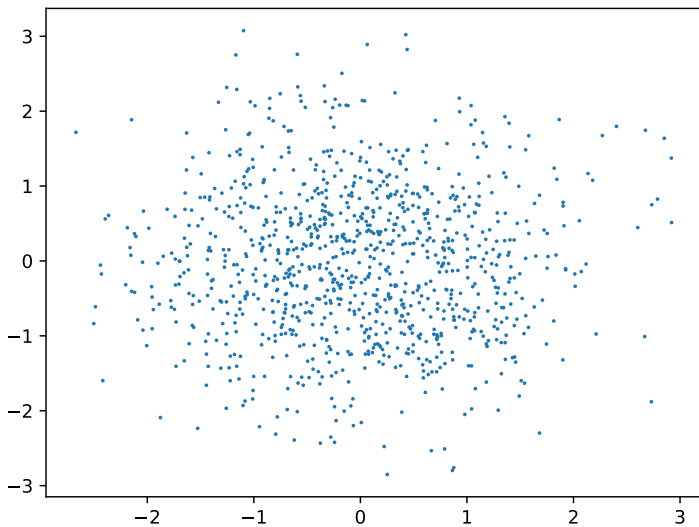
## Example 5

```
import numpy as np
import matplotlib.pyplot as plt

n = 1024
X = np.random.normal(0,1,n)
Y = np.random.normal(0,1,n)

plt.scatter(X,Y,s=1)
plt.savefig("figure5.pdf")
```

# Example 5



## Example 6

```
import numpy as np
import matplotlib.pyplot as plt

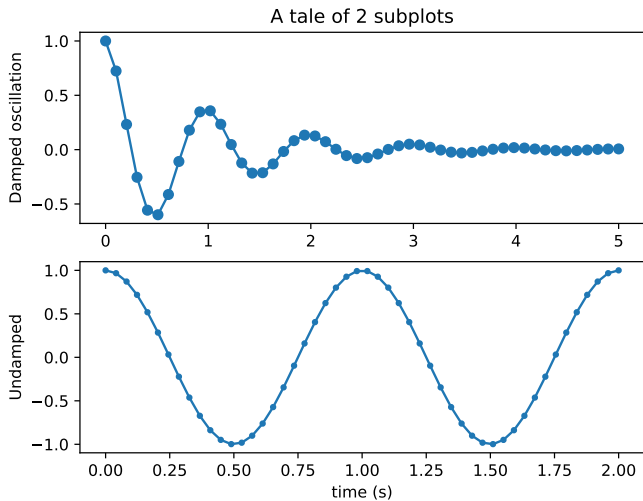
x1 = np.linspace(0.0, 5.0)
x2 = np.linspace(0.0, 2.0)
y1 = np.cos(2 * np.pi * x1) * np.exp(-x1)
y2 = np.cos(2 * np.pi * x2)

plt.subplot(2, 1, 1)
plt.plot(x1, y1, 'o-')
plt.title('A tale of 2 subplots')
plt.ylabel('Damped oscillation')

plt.subplot(2, 1, 2)
plt.plot(x2, y2, '-.')
plt.xlabel('time (s)')
plt.ylabel('Undamped')

plt.savefig("figure6.pdf")
```

# Example 6



# Tutorials

<http://www.labri.fr/perso/nrougier/teaching/matplotlib/>  
[http://journals.plos.org/ploscompbiol/article?id=10.1371/  
journal.pcbi.1003833](http://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1003833)