Sixth Semester Computer Science and Engineering
Open Lab: Python for Machine Learning
Lab sheet 3 Tutorial on Numpy

Numpy

Numpy is the core library for scientific computing in Python. It provides a high-performance multidimensional array object, and tools for working with these arrays. If you are already familiar with MATLAB, you might find this tutorial useful to get started with Numpy.

To use Numpy, we first need to import the `numpy` package:

```
import numpy as np
```

Arrays

A numpy array is a grid of values, all of the same type, and is indexed by a tuple of nonnegative integers. The number of dimensions is the rank of the array; the shape of an array is a tuple of integers giving the size of the array along each dimension.

We can initialize numpy arrays from nested Python lists, and access elements using square brackets:

```
a = np.array([1, 2, 3])  # Create a rank 1 array
print type(a), a.shape, a[0], a[1], a[2]
a[0] = 5                 # Change an element of the array
print a
```

```
<type 'numpy.ndarray'> (3,) 1 2 3
[5 2 3]
```

```
b = np.array([[1,2,3],[4,5,6]])   # Create a rank 2 array
print b
```

```
[[1 2 3]
 [4 5 6]]
```

```
print b.shape
print b[0, 0], b[0, 1], b[1, 0]
```

```
(2, 3)
1 2 4
```

Numpy also provides many functions to create arrays:

```
a = np.zeros((2,2))  # Create an array of all zeros
print a
```

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

```
b = np.ones((1,2))   # Create an array of all ones
print b
```

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

```
c = np.full((2,2), 7) # Create a constant array
print c
```

```
d = np.eye(2)        # Create a 2x2 identity matrix
print d
```

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

```
e = np.random.random((2,2)) # Create an array filled with random values
print e
```

```
[[ 0.09477679  0.79267634]
 [ 0.78291274  0.38962829]]
```

Array indexing

Numpy offers several ways to index into arrays.

Slicing: Similar to Python lists, numpy arrays can be sliced. Since arrays may be multidimensional, you must specify a slice for each dimension of the array:

```
import numpy as np

# Create the following rank 2 array with shape (3, 4)
# [[ 1  2  3  4]
#  [ 5  6  7  8]
#  [ 9 10 11 12]]
a = np.array([[1,2,3,4], [5,6,7,8], [9,10,11,12]])

# Use slicing to pull out the subarray consisting of the first 2 rows
# and columns 1 and 2; b is the following array of shape (2, 2):
# [[2 3]
#  [6 7]]
b = a[:2, 1:3]
print b
```

```
[[2 3]
 [6 7]]
```

A slice of an array is a view into the same data, so modifying it will modify the original array.

```
print a[0, 1]
b[0, 0] = 77    # b[0, 0] is the same piece of data as a[0, 1]
print a[0, 1]
```

```
2
77
```

You can also mix integer indexing with slice indexing. However, doing so will yield an array of lower rank than the original array. Note that this is quite different from the way that MATLAB handles array slicing:

```
# Create the following rank 2 array with shape (3, 4)
a = np.array([[1,2,3,4], [5,6,7,8], [9,10,11,12]])
print a
```

```
[[ 1  2  3  4]
 [ 5  6  7  8]
 [ 9 10 11 12]]
```

Two ways of accessing the data in the middle row of the array. Mixing integer indexing with slices yields an array of lower rank, while using only slices yields an array of the same rank as the original array:

```
row_r1 = a[1, :]    # Rank 1 view of the second row of a
row_r2 = a[1:2, :]  # Rank 2 view of the second row of a
row_r3 = a[[1], :]  # Rank 2 view of the second row of a
print row_r1, row_r1.shape
print row_r2, row_r2.shape
print row_r3, row_r3.shape
```

```
[ 4  5 26] (3,)
[[ 4  5 26]] (1, 3)
[[ 4  5 26]] (1, 3)
```

```
# We can make the same distinction when accessing columns of an array:
col_r1 = a[:, 1]
col_r2 = a[:, 1:2]
print col_r1, col_r1.shape
print
print col_r2, col_r2.shape
```

```
[ 2  6 10] (3,)

[[ 2]
 [ 6]
 [10]] (3, 1)
```

Integer array indexing: When you index into numpy arrays using slicing, the resulting array view will always be a subarray of the original array. In contrast, integer array indexing allows you to construct arbitrary arrays using the data from another array. Here is an example:

```
a = np.array([[1,2], [3, 4], [5, 6]])

# An example of integer array indexing.
# The returned array will have shape (3,) and
print a[[0, 1, 2], [0, 1, 0]]

# The above example of integer array indexing is equivalent to this:
print np.array([a[0, 0], a[1, 1], a[2, 0]])
```

```
[1 4 5]
[1 4 5]
```

```
# When using integer array indexing, you can reuse the same
# element from the source array:
print a[[0, 0], [1, 1]]
```

```
# Create a new array from which we will select elements
a = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
print a
```

```
[[ 1  2  3]
 [ 4  5  6]
 [ 7  8  9]
 [10 11 12]]
```

```
# Create an array of indices
b = np.array([0, 2, 0, 1])

# Select one element from each row of a using the indices in b
print a[np.arange(4), b]  # Prints "[ 1  6  7 11]"
```

```
[ 1  6  7 11]
```

```
# Mutate one element from each row of a using the indices in b
a[np.arange(4), b] += 10
print a
```

```
[[11  2  3]
 [ 4  5 16]
 [17  8  9]
 [10 21 12]]
```

Boolean array indexing: Boolean array indexing lets you pick out arbitrary elements of an array. Frequently this type of indexing is used to select the elements of an array that satisfy some condition. Here is an example:

```
import numpy as np

a = np.array([[1,2], [3, 4], [5, 6]])

bool_idx = (a > 2)  # Find the elements of a that are bigger than 2;
                    # this returns a numpy array of Booleans of the same
                    # shape as a, where each slot of bool_idx tells
                    # whether that element of a is > 2.

print bool_idx
```

```
[[False False]
 [ True  True]
 [ True  True]]
```

```
# We use boolean array indexing to construct a rank 1 array
# consisting of the elements of a corresponding to the True values
# of bool_idx
print a[bool_idx]

# We can do all of the above in a single concise statement:
print a[a > 2]
```

```
[3 4 5 6]
[3 4 5 6]
```

Datatypes

Every numpy array is a grid of elements of the same type. Numpy provides a large set of numeric datatypes that you can use to construct arrays. Numpy tries to guess a datatype when you create an array, but functions that construct arrays usually also include an optional argument to explicitly specify the datatype. Here is an example:

```
x = np.array([1, 2])  # Let numpy choose the datatype
y = np.array([1.0, 2.0])  # Let numpy choose the datatype
z = np.array([1, 2], dtype=np.int64)  # Force a particular datatype

print x.dtype, y.dtype, z.dtype
```

```
int64 float64 int64
```

You can read all about numpy datatypes in the documentation.

Array math

Basic mathematical functions operate elementwise on arrays, and are available both as operator overloads and as functions in the numpy module:

```
x = np.array([[1,2],[3,4]], dtype=np.float64)
y = np.array([[5,6],[7,8]], dtype=np.float64)

# Elementwise sum; both produce the array
print x + y
print np.add(x, y)
```

```
[[  6.   8.]
 [ 10.  12.]]
[[  6.   8.]
 [ 10.  12.]]
```

```
# Elementwise difference; both produce the array
print x - y
print np.subtract(x, y)
```

```
[[-4. -4.]
 [-4. -4.]]
[[-4. -4.]
 [-4. -4.]]
```

```
# Elementwise product; both produce the array
print x * y
print np.multiply(x, y)
```

```
[[  5.  12.]
 [ 21.  32.]]
[[  5.  12.]
 [ 21.  32.]]
```

```
# Elementwise division; both produce the array
# [[ 0.2         0.33333333]
#  [ 0.42857143  0.5       ]]
print x / y
print np.divide(x, y)
```

```
[[ 0.2         0.33333333]
 [ 0.42857143  0.5       ]]
[[ 0.2         0.33333333]
 [ 0.42857143  0.5       ]]
```

```
# Elementwise square root; produces the array
# [[ 1.          1.41421356]
#  [ 1.73205081  2.        ]]
print np.sqrt(x)
```

```
[[ 1.          1.41421356]
 [ 1.73205081  2.        ]]
```

Note that unlike MATLAB, * is elementwise multiplication, not matrix multiplication. We instead use the dot function to compute inner products of vectors, to multiply a vector by a matrix, and to multiply matrices. dot is available both as a function in the numpy module and as an instance method of array objects:

```
x = np.array([[1,2],[3,4]])
y = np.array([[5,6],[7,8]])

v = np.array([9,10])
w = np.array([11, 12])

# Inner product of vectors; both produce 219
print v.dot(w)
print np.dot(v, w)
```

```
219
219
```

```
# Matrix / vector product; both produce the rank 1 array [29 67]
print x.dot(v)
print np.dot(x, v)
```

```
[29 67]
[29 67]
```

```
# Matrix / matrix product; both produce the rank 2 array
# [[19 22]
#  [43 50]]
print x.dot(y)
print np.dot(x, y)
```

```
[[19 22]
 [43 50]]
[[19 22]
 [43 50]]
```

```
x = np.array([[1,2],[3,4]])

print np.sum(x)  # Compute sum of all elements; prints "10"
print np.sum(x, axis=0)  # Compute sum of each column; prints "[4 6]"
print np.sum(x, axis=1)  # Compute sum of each row; prints "[3 7]"
```

```
10
[4 6]
[3 7]
```

You can find the full list of mathematical functions provided by numpy in the documentation.

Apart from computing mathematical functions using arrays, we frequently need to reshape or otherwise manipulate data in arrays. The simplest example of this type of operation is transposing a matrix; to transpose a matrix, simply use the T attribute of an array object:

```
print x
print x.T
```

```
[[1 2]
 [3 4]]
[[1 3]
 [2 4]]
```

```
v = np.array([[1,2,3]])
print v
print v.T
```

```
[1 2 3]
[1 2 3]
```

Broadcasting

Broadcasting is a powerful mechanism that allows numpy to work with arrays of different shapes when performing arithmetic operations. Frequently we have a smaller array and a larger array, and we want to use the smaller array multiple times to perform some operation on the larger array.

For example, suppose that we want to add a constant vector to each row of a matrix. We could do it like this:

```
# We will add the vector v to each row of the matrix x,
# storing the result in the matrix y
x = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
v = np.array([1, 0, 1])
y = np.empty_like(x)   # Create an empty matrix with the same shape as x

# Add the vector v to each row of the matrix x with an explicit loop
for i in range(4):
    y[i, :] = x[i, :] + v

print y
```

```
[[ 2  2  4]
 [ 5  5  7]
 [ 8  8 10]
 [11 11 13]]
```

This works; however when the matrix x is very large, computing an explicit loop in Python could be slow. Note that adding the vector v to each row of the matrix x is equivalent to forming a matrix vv by stacking multiple copies of v vertically, then performing elementwise summation of x and vv. We could implement this approach like this:

```
vv = np.tile(v, (4, 1))  # Stack 4 copies of v on top of each other
print vv                 # Prints "[[1 0 1]
                         #         [1 0 1]
                         #         [1 0 1]
                         #         [1 0 1]]"
```

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

```
y = x + vv  # Add x and vv elementwise
print y
```

```
[[ 2  2  4]
 [ 5  5  7]
 [ 8  8 10]
 [11 11 13]]
```

Numpy broadcasting allows us to perform this computation without actually creating multiple copies of v. Consider this version, using broadcasting:

```
import numpy as np

# We will add the vector v to each row of the matrix x,
# storing the result in the matrix y
x = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
v = np.array([1, 0, 1])
y = x + v  # Add v to each row of x using broadcasting
print y
```

```
[[ 2  2  4]
 [ 5  5  7]
 [ 8  8 10]
 [11 11 13]]
```

```
# Compute outer product of vectors
v = np.array([1,2,3])  # v has shape (3,)
w = np.array([4,5])    # w has shape (2,)
# To compute an outer product, we first reshape v to be a column
# vector of shape (3, 1); we can then broadcast it against w to yield
# an output of shape (3, 2), which is the outer product of v and w:

print np.reshape(v, (3, 1)) * w
```

```
[[ 4  5]
 [ 8 10]
 [12 15]]
```

```
# Add a vector to each row of a matrix
x = np.array([[1,2,3], [4,5,6]])
# x has shape (2, 3) and v has shape (3,) so they broadcast to (2, 3),
# giving the following matrix:

print x + v
```

```
[[2 4 6]
 [5 7 9]]
```

```
# Add a vector to each column of a matrix
# x has shape (2, 3) and w has shape (2,).
# If we transpose x then it has shape (3, 2) and can be broadcast
# against w to yield a result of shape (3, 2); transposing this result
# yields the final result of shape (2, 3) which is the matrix x with
# the vector w added to each column. Gives the following matrix:

print (x.T + w).T
```

```
[[ 5  6  7]
 [ 9 10 11]]
```

```
# Another solution is to reshape w to be a row vector of shape (2, 1);
# we can then broadcast it directly against x to produce the same
# output.
print x + np.reshape(w, (2, 1))
```

```
[[ 5  6  7]
 [ 9 10 11]]
```

```
# Multiply a matrix by a constant:
# x has shape (2, 3). Numpy treats scalars as arrays of shape ();
# these can be broadcast together to shape (2, 3), producing the
# following array:
print x * 2
```

```
[[ 2  4  6]
 [ 8 10 12]]
```

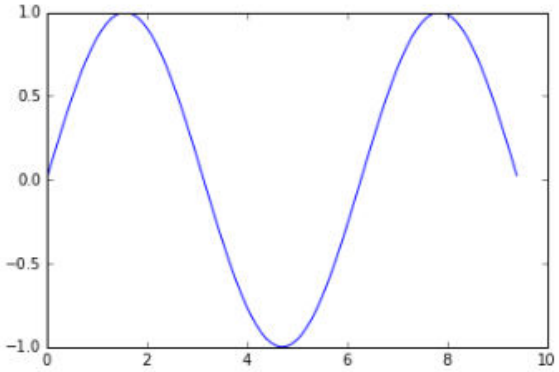
Plotting

The most important function in `matplotlib` is plot, which allows you to plot 2D data. Here is a simple example:

```
# Compute the x and y coordinates for points on a sine curve
x = np.arange(0, 3 * np.pi, 0.1)
y = np.sin(x)

# Plot the points using matplotlib
plt.plot(x, y)
```

```
[<matplotlib.lines.Line2D at 0x112d11710>]
```

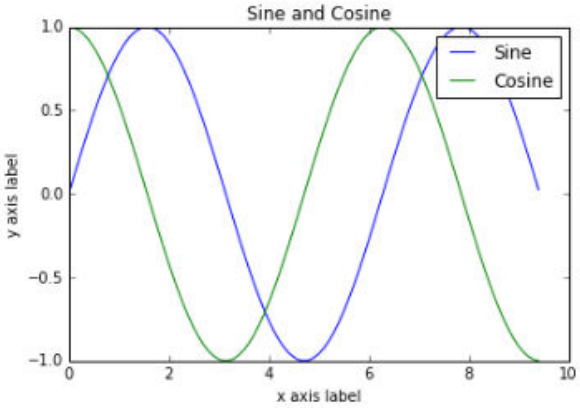


With just a little bit of extra work we can easily plot multiple lines at once, and add a title, legend, and axis labels:

```
y_sin = np.sin(x)
y_cos = np.cos(x)

# Plot the points using matplotlib
plt.plot(x, y_sin)
plt.plot(x, y_cos)
plt.xlabel('x axis label')
plt.ylabel('y axis label')
plt.title('Sine and Cosine')
plt.legend(['Sine', 'Cosine'])
```

```
<matplotlib.legend.Legend at 0x11739ac50>
```



Subplots

You can plot different things in the same figure using the subplot function. Here is an example:

```
# Compute the x and y coordinates for points on sine and cosine curves
x = np.arange(0, 3 * np.pi, 0.1)
y_sin = np.sin(x)
y_cos = np.cos(x)

# Set up a subplot grid that has height 2 and width 1,
# and set the first such subplot as active.
plt.subplot(2, 1, 1)

# Make the first plot
plt.plot(x, y_sin)
plt.title('Sine')

# Set the second subplot as active, and make the second plot.
plt.subplot(2, 1, 2)
plt.plot(x, y_cos)
plt.title('Cosine')

# Show the figure.
plt.show()
```