# → Aman's Al Journal | Primers | NumPy Tutorial

## Overview

- NumPy is the core library for scientific computing in Python. It is informally known as the the swiss army knife of the data scientist.
- It provides a high-performance multidimensional array object numpy.ndarray, and tools for operating on these arrays.
- If you're already familiar with numerical processing in a different language like MATLAB and R, here are some recommended references:
  - NumPy for MATLAB users
  - Python for R users
- Related primers: Matplotlib and SciPy.

# Arrays

- A NumPy array is a grid of values, all of the same type, and is indexed by a tuple of non-negative 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) lists and tuples, and access elements using square brackets as array subscripts:

```
import numpy as np
                                     # Define a rank 1 array using a list
a = np.array([1, 2, 3])
print(type(a))
                                     # Prints <class 'numpy.ndarray'>
print(a.shape)
                                     # Prints (3,)
print(a[0], a[1], a[2])
                                     # Prints (1, 2, 3)
a[0] = 5
                                     # Change an element of the array
                                     # Prints [5 2 3]
print(a)
b = np.array([[1, 2, 3]])
                                     # Define a rank 2 array (vector) using a nested list
print(b.shape)
                                     # Prints (1, 3)
```

```
c = np.array([[1, 2, 3], [4, 5, 6]]) # Define a rank 2 array (matrix) using a nested list
print(c.shape)
                                   # Prints (2, 3)
print(c[0, 0], c[0, 1], c[1, 0]) # Prints (1, 2, 4)
                           # Define a rank 1 array from a tuple using a nested list
d = np.array((1, 2, 3))
                                # Prints [1 2 3]
print(d)
                                   # Prints (3,)
print(d.shape)
e = np.array(((1, 2, 3), (4, 5, 6))) # Define a rank 2 array using a nested list
print(e)
                                     # Prints [[1, 2, 3],
                                               [4, 5, 6]]
# NumPy arrays can be initialized using other NumPy arrays or lists
# but note that the resulting matrix is always of type NumPy ndarray
                                    # Define a python list
1 = [1, 2, 3]
a = np.array([1, 2, 3]) # Define a numpy array by passing in a list
f = np.array([a, a, a])  # Matrix initialized with NumPy arrays
g = np.array([l, l, l])  # Matrix initialized with lists
h = np.array([a, [1, 1, 1], a]) # Matrix initialized with both types
# All the below statements print [[1 2 3]
#
                                  [1 2 3]
                                  [1 2 3]]
print(f)
print(g)
print(h)
```

• Note the difference between a Python list and a NumPy array. NumPy arrays are designed for numerical (vector/matrix) operations, while lists are for more general purposes.

```
import numpy as np

l = [1, 2, 3]  # Define a python list
a = np.array([1, 2, 3]) # Define a numpy array by passing in a list
print(l)  # Prints [1, 2, 3]
```

```
print(a)  # Prints [1 2 3]

print(type(l))  # Prints <class 'list'>
print(type(a))  # Prints <class 'numpy.ndarray'>
```

Note that when defining an array, be sure that all the rows contain the same number of columns/elements. Otherwise, algebraic
operations on malformed matrices could lead to unexpected results:

• NumPy also provides many functions to create arrays:

```
# Define an array of all ones
b = np.ones((1, 2))
                                            # Prints [[ 1. 1.]]
print(b)
c = np.full((2, 2), 7)
                                            # Define a constant array
print(c)
                                            # Prints [[ 7. 7.]
                                                [ 7. 7.]]
                                            # Define a 2x2 identity matrix
d = np.eve(2)
print(d)
                                            # Prints [[ 1. 0.]
                                                 [ 0. 1.]]
                                           # Define a 2x2 matrix from the uniform distribution [0, 1)
e = np.random.random((2, 2))
                                            # Prints a 2x2 matrix of random values
print(e)
g = 5 * np.random.random sample((2, 2)) - 5 # Sample 2x2 matrix from Unif[-5, 0)
                                           # Sample from Unif[a, b), b > a: (b - a) * random sample() + a
                                            # Prints a 2x2 matrix of random values
print(f)
f = np.random.randn(2, 2)
                                           # Sample a 2x2 matrix from the "standard normal" distribution
print(f)
                                            # Prints a 2x2 matrix of random values
g = 2.5 * np.random.randn(2, 2) + 3
                                           # Sample 2x2 matrix from N(mean=3, var=6.25)
                                           # General form: stddev * np.random.randn(...) + mean
print(f)
                                            # Prints a 2x2 matrix of random values
```

- Note that with np.random.randn(), the length of each dimension of the output array is an **individual argument**. On the other hand, np.random.random() accepts its shape argument as a **single tuple containing all dimensions**. More on this in the section on <u>standard</u> normal.
- You can read about other methods of array creation in the NumPy documentation.

# Array indexing

• NumPy offers several ways to index into arrays.

# Row and column indexing

• To "select" a particular row or column in an array, NumPy offers similar functionality as Python lists:

• You can use np.arange() to select the rows/columns of an array. For more details on np.arange(), refer to the section on arrange below.

• You can use an "index-array" that contains indices of rows or columns to index into another array. This is a very common use-case in NumPy-based projects.

```
import numpy as np
```

```
a = np.array([[1, 2], [3, 4]])
# Selecting columns using an index array
b = [0, 0]
            # Select the first column for both rows (see below)
a[np.arange(1), b] # Prints [1, 1] (same as a[0, b])
a[np.arange(2), b] # Prints [1, 3] (same as a[[0, 1], b])
a[:, b]
                  # Prints [[1, 1],
                            [3, 3]]
# Selecting rows using an index array
                  # Select the first row for both columns (see below)
b = [0, 0]
a[b, np.arange(1)] # Prints [1, 1] (same as a[b, 0])
a[b, np.arange(2)] # Prints [1, 2] (same as a[b, [0, 1]])
a[b, :]
                  # Prints [[1, 2],
                         [1, 2]]
```

### ▼ 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

# Define 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]

# A slice of an array is a view into the same data, so modifying it
# will modify the original array
print(a[0, 1]) # Prints 2
b[0, 0] = 77  # b[0, 0] is the same piece of data as a[0, 1]
print(a[0, 1]) # Prints 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:

```
import numpy as np
# Define 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]])
# 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
# Prints [[5 6 7 8]] (1, 4)
print(row r2, row r2.shape)
# We can make the same distinction when accessing columns of an array:
col_r1 = a[:, 1]
col r2 = a[:, 1:2]
print(col_r2, col_r2.shape)
                                # Prints [[ 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:

```
import numpy as np

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]])  # Prints [1 4 5]

# The above example of integer array indexing is equivalent to this:
print(np.array([a[0, 0], a[1, 1], a[2, 0]]))  # Prints [1 4 5]

# When using integer array indexing, you can reuse the same
# element from the source array:
print(a[[0, 0], [1, 1]])  # Prints [2 2]

# Equivalent to the previous integer array indexing example
print(np.array([a[0, 1], a[0, 1]]))  # Prints [2 2]
```

• One useful trick with integer array indexing is selecting or mutating one element from each row of a matrix:

```
import numpy as np
# Define 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)
                          # Prints [[ 1, 2, 3],
                                   [4, 5, 6],
                                   [7, 8, 9],
                                   [10, 11, 12]]
# Define 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]
# Mutate one element from each row of a using the indices in b
a[np.arange(4), b] += 10
print(a)
                          # Prints [[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]])
```

```
print(a[True]) # Same as print(a), interpreted as a "True" mask
                  # on each of a's elements
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)
                  # Prints [[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]) # Prints [3 4 5 6]
# We can do all of the above in a single concise statement:
print(a[a > 2]) # Prints [3 4 5 6]
```

• As an extension of the above concept, to select elements on an array based on the elements of another array:

```
import numpy as np

a = np.array([1, 2, 3, 4, 5, 6])
b = np.array(['f','o','o','b','a','r'])

# Note that & is the bitwise AND operator, and && is not supported in NumPy,
# so np.logical_and() is used in the below example
print(b[np.logical_and((a > 1), (a < 5))]) # Prints ['o','o','b']

# Another way to accomplish this is using np.all(),
# which is explained in the section on "all" below.
print(b[np.all([a > 1, a < 5], axis=0)]) # Prints ['o','o','b']</pre>
```

• For brevity, we have left out a lot of details about NumPy array indexing; if you want to know more you should read the <u>NumPy</u> documentation.

# 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.
- As an example:

```
[ ] Ļ1 cell hidden
```

• You can read all about datatypes in the NumPy documentation.

# Array math

NumPy provides many functions for manipulating arrays; you can find an exhaustive list in the <u>NumPy documentation</u>. Some common ones are listed below.

## Element-wise operations

• Algebraic operations such as +, -, \*, / etc. are available both as operator overloads and as functions in the NumPy module. These operators carry out **element-wise** operations on NumPy arrays:

```
import numpy as np

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
```

```
10/1/22, 9:24 AM
   # [[ 6.0 8.0]
   # [10.0 12.0]]
   print(x + y)
   print(np.add(x, y))
   # Elementwise difference; both produce the array
   # [[-4.0 -4.0]
   # [-4.0 -4.0]]
   print(x - y)
   print(np.subtract(x, y))
   # Elementwise product; both produce the array
   # [[ 5.0 12.0]
   # [21.0 32.0]]
   print(x * y)
   print(np.multiply(x, y))
   # Elementwise division; both produce the array
   # [[ 0.2
                    0.33333333]
   # [ 0.42857143 0.5
                             11
   print(x / y)
   print(np.divide(x, y))
   # Elementwise square root; produces the array
   # [[ 1.
           1.41421356]
   # [ 1.73205081 2.
```

### ▼ NumPy arrays vs. Python lists

print(np.sqrt(x))

- A common mistake is to mix up the concepts of NumPy arrays and Python lists.
- Note that the + operator in the context of NumPy arrays performs an **element-wise addition**, while the same operation on Python lists results in a **list extension**.

- With NumPy arrays, we can **scale** the vector with \* by performing **element-wise multiplication**, while the same operation on Python lists results in a **list concatenation** (and in MATLAB, results in **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. We discuss this in detail in the section on dot product below.

- Make note of this while coding since a function can utilize both Python lists and NumPy arrays. Knowing this can save many headaches!
- Scaling and translating arrays
  - Using regular algebraic operators like + and that we saw in the prior section on <u>element-wise operations</u>, we can scale and translate/shift NumPy arrays.
  - Operations can be performed between:
    - Two NumPy arrays or,
    - NumPy arrays and scalars.

```
import numpy as np
```

#### ▼ Norm

• NumPy offers a set of algebraic functions in the class **linalg**, which includes the **norm** function:

```
import numpy as np
a = np.array([1, 2, 3, 4])  # Define an array
norm1 = np.linalg.norm(a)

a = np.array([[1, 2], [3, 4]]) # Define a 2x2 matrix
norm2 = np.linalg.norm(a)

# Both print 5.477225575051661
print(norm1)
print(norm2)
```

- By default, np.linalg.norm() calculates the **Frobenius norm** for matrices and the **2-norm** for vectors, unless the ord argument is overridden.
  - Recall from linear algebra that the norm (or magnitude) of an n-dimensional vector v is the square root of the sum of its elements
     squared:

- Also, the \*\*Frobenius norm\*\* is the generalization of the vector norm for matrices, and is defined for a matrix \\(A\\) as:

```
\ \|\mathrm{A}\\|_{F} = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n}\left|a_{i j}\right^{2}} $$
```

• The following code snippet compares a manual implementation of the norm vs. the np.linalg.norm() function. Both yield the same result.

```
import numpy as np
a = np.array([[1, 2], [3, 4]]) # Define a 2x2 matrix
norm = np.sqrt(np.sum(np.square(a)))

# Both should yield the same result and print:
# 5.477225575051661 == 5.477225575051661
print(norm, '== ', np.linalg.norm(a))

a = np.array([1, 2, 3, 4]) # Define an array
norm = np.sqrt(np.sum(np.square(a)))

# Both should yield the same result and print:
# 5.477225575051661 == 5.477225575051661
print(norm, '== ', np.linalg.norm(a))
```

- Note that if the axis argument to np.linalg.norm() is not explicitly specified, the function defaults to treating the matrix as a "flat" array of numbers implying that it takes every element of the matrix into account. However, it is possible to get the a row-wise or column-wise norm using the axis parameter:
  - o axis=0 operates across all rows, i.e., gets the norm of each **column**.
  - o axis=1 operates across all columns, i.e., gets the norm of each row.

```
import numpy as np

a = np.array([[1, 1], [2, 2], [3, 3]]) # Define a 3x2 matrix

normByCols = np.linalg.norm(a, axis=0) # Get the norm for each column; returns 2 elements
normByRows = np.linalg.norm(a, axis=1) # get the norm for each row; returns 3 elements

print(normByCols) # [3.74165739 3.74165739]
print(normByRows) # [1.41421356 2.82842712 4.24264069]
```

### ▼ Dot product

• Dot product is available both as a function in the NumPy module np.dot() and as an instance method of array objects <ndarray>.dot():

```
import numpy as np
x = np.array([[1, 2], [3, 4]])
y = np.array([[5, 6], [7, 8]])
v = np.array([9, 10])
w = np.array([11, 12])
# Dot/scalar/inner product of vectors; both produce a scalar: 219
print(v.dot(w))
print(np.dot(v, w))
# Matrix/vector product; both produce the rank 1 array [29 67]
print(x.dot(v))
print(np.dot(x, v))
# Matrix/matrix product; both produce the rank 2 array
# [[19 22]
# [43 50]]
print(x.dot(y))
print(np.dot(x, y))
```

• Some alternative ways to obtain the dot product:

```
import numpy as np

print(np.sum(v * w)) # Using the definition of dot product

print(v @ w)  # numpy>=1.10 overloads the new Pythonic operator "@" for dot product

# Inefficient, unrolled, non-vectorized implementation
dotProduct = 0
for a, b in zip(v, w):
    dotProduct += a * b

print(dotProduct)
```

• np.dot() is strongly recommended since it accepts both NumPy arrays and Python lists:

```
import numpy as np

n1 = np.dot(np.array([1, 2]), np.array([3, 4])) # Dot product on numpy arrays
n2 = np.dot([1, 2], [3, 4]) # Dot product on python lists

# Both print 11
print(n1)
print(n2)
```

# 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.

- Broadcasting typically makes your code more concise and faster, so you should strive to use it where possible.
- The simplest broadcasting example occurs when an array and a scalar value are combined in an operation:

```
import numpy as np

a = np.array([1, 2, 3])
b = 2
print(a * b) # Prints [ 2, 4, 6]

# Note that the result is equivalent to the next example where b is an array!
a = np.array([1, 2, 3])
b = np.array([2, 2, 2])
print(a * b) # Prints [ 2, 4, 6]
```

• Consider another example where we'd like to add a constant vector to each row of a matrix. We could do it like this:

```
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 = np.empty_like(x)  # Define 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

# Now y is the following
# [[ 2  2  4]
#  [ 5  5  7]
#  [ 8  8  10]
#  [11  11  13]]
print(y)
```

- 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 element-wise summation of x and vv. We could implement this approach like this:

```
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])
vv = np.tile(v, (4, 1)) # Stack 4 copies of v on top of each other
                       # Prints [[1 0 1]
print(vv)
                                 [1 0 1]
                                 [1 0 1]
                                 [1 0 1]]
                       # Add x and vv element-wise
V = X + VV
print(v)
                       # Prints [[ 2 2 4
                               [557]
                                 [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:

• The line y = x + v works even though x has shape (4, 3) and v has shape (3,) due to broadcasting; this line works as if v actually had shape (4, 3), where each row was a copy of v, and the sum was performed element-wise.

#### ▼ Rules

- Broadcasting two arrays together follows these rules:
  - If the arrays do not have the same rank, prepend the shape of the lower rank array with ones until both shapes have the same length.
    - This implies that the arrays do not need to have the same number of dimensions.
  - If the arrays have the same rank, NumPy compares their shapes element-wise. It starts with the trailing dimensions and works its
    way forward, checking if the arrays are compatible in every dimension, as follows:
    - The two arrays are said to be compatible in a dimension if:
      - They have the same size in the dimension or,
      - One of the arrays has size 1 in that dimension.
    - The arrays can only be broadcast together if they are compatible in all dimensions.
    - When either of the dimensions belonging to both arrays being compared is 1, the **other** is used. In other words, dimensions with size 1 are **stretched or "copied"** to match the other. This is the **primary broadcasting** step.
    - After broadcasting, each array behaves as if it its shape is now equal to the element-wise maximum of shapes of the two input arrays.
- Functions that support broadcasting are known as **universal functions**. You can find an exhaustive list of universal functions in the <a href="NumPy documentation">NumPy documentation</a>.

## Examples

• Examples from NumPy's documentation on Broadcasting:

```
1. **Either array has axes with length 1**: In the following example, array \(B\\) has an axis with length \(1\\).
    - To tackle an axis with length \\(1\\) during broadcasting, we simply expand that dimension to match the other array's.
    . . .
           (3d array): 15 x 3 x 5
    Α
           (3d array): 15 \times 1 \times 5
    Result (3d array): 15 \times 3 \times 5
1. **Both arrays have axes with length 1**: In the following example, arrays \(A\) and \(B\) both have axes with length \(1\).
    - Extrapolating the case above, to tackle an axis with length \\(1\\) in either array during broadcasting, we simply expand that
           (4d array): 8 x 1 x 6 x 1
           (3d array): 7 x 1 x 5
    Result (4d array): 8 \times 7 \times 6 \times 5
1. **Rank mismatch**: In the following example, arrays \(A\) and \(B\) do not have the same rank.
    - Recall that to tackle rank mismatch during broadcasting, we prepend the shape of the lower rank array with ones until both shap
    . . .
           (2d array): 5 x 4
           (1d array): 4
    Result (2d array): 5 x 4
           (3d array): 15 \times 3 \times 5
           (2d array): 3 x 5
    Result (3d array): 15 \times 3 \times 5
```

. . .

```
A (3d array): 256 x 256 x 3
B (1d array): 3
Result (3d array): 256 x 256 x 3
```

1. \*\*Rank mismatch and axes with length 1\*\*: In the following example, arrays \\(A\\) and \\(B\\) do not have the same rank and \\(B\\) - Tackling rank mismatch was discussed in example \\(3\\). Also, handling an axis with length \\(1\\) was discussed in example \\

```
A (2d array): 5 x 4
B (1d array): 1
Result (2d array): 5 x 4

A (3d array): 15 x 3 x 5
B (2d array): 3 x 1
Result (3d array): 15 x 3 x 5
```

- Some examples that do not broadcast:
- 1. \*\*Dimension mismatch\*\*: In the following example, arrays \\(A\\) and \\(B\\) are not compatible in each dimension and thus, cannot Recall that the two arrays need to be \*\*compatible\*\* in each dimension (starting from the trailing dimension) for broadcasting

```
A (1d array): 3
B (1d array): 4  # Trailing dimensions do not match

A (2d array): 2 x 1
B (3d array): 8 x 4 x 3 # Second from last dimensions mismatched
```

Broadcasting examples in code:

```
import numpy as np
# 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:
# [[ 4 5]
# [ 8 10]
# [12 15]]
print(np.reshape(v, (3, 1)) * w)
# Note that np.reshape() is described in detail in the section on "reshape" below.
# 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:
# [[2 4 6]
# [5 7 9]]
print(x + v)
# 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:
# [[ 5 6 7]
# [ 9 10 11]]
print((x.T + w).T)
# Another solution is to reshape w to be a column 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)))

# 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:
# [[ 2  4  6]
# [ 8 10 12]]
print(x * 2)
```

# Data centering

• In some scenarios, centering the elements of a dataset is an important preprocessing step. Centering a dataset involves **subtracting the mean from the data**. The resultant data is called zero-centered, since the mean of the resultant dataset is 0.

## Column-centering

• Column-centering a matrix involves subtracting the column mean from each element within a particular column. Note that the sum by columns of a centered matrix is always 0.

```
import numpy as np
a = np.array([[1, 1], [2, 2], [3, 3]]) # Define a 3x2 matrix.

centered = a - np.mean(a, axis=0) # Remove the mean for each column

# Column-centered matrix
print(centered) # Prints [[-1. -1.]
# [ 0.  0.]
# [ 1.  1.]]

# New mean-by-column should be 0
print(centered.mean(axis=0)) # Prints [0. 0.]
```

### ▼ Row-centering

• For row centering, transpose the matrix, center by columns, and then transpose back the result.

```
import numpy as np
a = np.array([[1, 3], [2, 4], [3, 5]]) # Define a 3x2 matrix.

centered = a.T - np.mean(a, axis=1) # Remove the mean for each row centered = centered.T # Transpose back the result

# Row-centered matrix
print(centered) # Prints [[-1. 1.]] # [-1. 1.]]

# New mean-by-rows should be 0
print(centered.mean(axis=1)) # Prints [0. 0. 0.]
```

### Selected functions

- NumPy provides a host of useful functions for performing computations on arrays. Below, we've touched upon some of the most useful ones that you'll encounter regularly in projects.
- You can find an exhaustive list of mathematical functions in the NumPy documentation.
- As discussed in the section on <u>norm</u>, most of these functions accept an axis parameter which when specified, performs the operation on a per-column (axis=0) or per-row basis (axis=1) rather than on the entire array.

#### Initialization

#### Random seed

• Provide a seed to the generator. Used to foster reproducibility of random numbers.

```
import numpy as np

np.random.seed(0) # Here, 0 is the seed.

a = np.random.rand()
print(a) # Print 0.5488135039273248

np.random.seed(0) # Set seed again for next random number to match the prior one.

a = np.random.rand()
print(a) # Print 0.5488135039273248
```

### ▼ Standard normal

- Return samples from the standard normal (also called the standard Gaussian) distribution.
- Note that np.random.randn() is a convenience function for users porting code from MATLAB, and wraps np.random.standard\_normal().

  As such, np.random.randn() takes dimensions as individual ints.
  - On the other hand, np.random.standard\_normal() takes a shape argument as a **tuple** to specify the size of the output, which is consistent with other NumPy functions like np.zeros() and np.ones().

```
import numpy as np

a = np.random.randn(2, 2)  # Sample a 2x2 matrix from the standard normal distribution
print(a)  # Prints a 2x2 matrix of random values

b = np.random.standard_normal((2, 2)) # Sample a 2x2 matrix from the standard normal distribution
print(b)  # Prints a 2x2 matrix of random values
```

• To sample the normal distribution  $a \sim \mathcal{N}(\mu, \sigma^2)$ , multiply the output of np.random.randn() by  $\sigma$  and add  $\mu$ , i.e., stddev \* np.random.randn(...) + mean}

#### ▼ Uniform

- Samples random floats from a continuous uniform distribution -- the half-open interval [0.0, 1.0).
- Note that np.random.rand() is a convenience function for users porting code from MATLAB, and wraps np.random.random(). As such, np.random.rand() takes **dimensions as individual ints**.
  - On the other hand, np.random.random() takes a shape argument as a **tuple** to specify the size of the output, which is consistent with other NumPy functions like np.zeros() and np.ones().

```
import numpy as np

a = np.random.rand(2, 2)  # Define a 2x2 matrix from the uniform distribution [0, 1)
print(a)  # Prints a 2x2 matrix of random values

b = np.random.random((2, 2)) # Define a 2x2 matrix from the uniform distribution [0, 1)
print(b)  # Prints a 2x2 matrix of random values
```

• To sample the uniform distribution  $a \sim Unif(x,y)$ , given y>x, Note that <code>np.random.uniform()</code> offers this functionality (drawing samples from a uniform distribution within an arbitrary range) much more directly by accepting three arguments: <code>low=0.0</code>, <code>high=1.0</code>, <code>size=None</code>. The following code snippet thus yields the same output as the one above.

```
import numpy as np
a = np.random.uniform(-5, 0, size=(2,2)) # Sample 2x2 matrix from Unif[-5, 0)
print(a) # Prints a 2x2 matrix of random values
```

• Note that np.random.random() also offers this functionality (drawing samples from a uniform distribution within an arbitrary range) by multiplying its output by (y - x) and adding x, i.e., (y - x) \* np.random.random(...) + x

• Without explicit arguments, the functions rand(), random(), uniform() and random\_sample() are equivalent, producing a random float in the range [0.0, 1.0).

```
import numpy as np

np.random.seed(0)

a = np.random.rand()
print(a)  # Print 0.5488135039273248

b = np.random.random()
print(b)  # Print 0.7151893663724195

c = np.random.uniform()
print(c)  # Print 0.6027633760716439

d = np.random.random_sample()  # numpy.random.random() is an alias for numpy.random.random_sample()
print(d)  # Print 0.5448831829968969
```

#### ▼ Random choice

• Generates a random sample from a given 1D array. The main arguments to np.random.choice() are a and size.

- o a can be an indarray, in which case a random sample is returned from its elements. If it's an int, the random sample is generated as if a were np.arange(a).
- o size is an optional argument that can hold an int or a tuple of ints. If it is not overriden, a single value is returned by default.

```
# Generate a uniform random sample from np.arange(5) of size 3
# This is equivalent to np.random.randint(0,5,3)
print(np.random.choice(5, 3))  # Prints [0 3 4]

# Generate a non-uniform random sample from np.arange(5) of size 3
print(np.random.choice(5, 3, p=[0.1, 0, 0.3, 0.6, 0])) # Prints [3 3 0]

# Generate a uniform random sample from np.arange(5) of size 3 without replacement
print(np.random.choice(5, 3, replace=False))  # Prints [4 1 3]
```

### → Arange

- Return evenly spaced values within the half-open interval [start, stop) (in other words, the interval including start but excluding stop).
- For integer arguments the function is equivalent to the Python built-in range function, but returns an ndarray rather than a list.

```
import numpy as np

print(np.arange(8))  # Prints [0 1 2 3 4 5 6 7]
print(np.arange(3, 8))  # Prints [3 4 5 6 7]
print(np.arange(3, 8, 2))  # Prints [3 5 7]
```

• When using a non-integer step, such as 0.1, the results will often not be consistent. It is better to use np.linspace() for those cases as below.

# ▼ Linspace

- Return evenly spaced numbers over a specified interval.
- Returns 50 evenly spaced samples (which can be overriden by num), calculated over the interval [start, stop].

### ▼ Reshape

- Gives a new shape to an array without changing its data.
- Note that np.reshape() returns a **view** of the array when the elements are contiguous in memory (just like <a href="np.ravel()">np.ravel()</a>). So modifying the result of np.reshape() would also modify the original array. However, np.reshape() returns a copy if, for e.g., the input array were made from slicing another array using a **non-unit** step size (e.g. a = x[::2]).

#### → -1 in Reshape

• NumPy allows us to assign **one** (and only one) value of the shape argument to a function as -1. NumPy figures out the unknown dimension by looking at the length of the array and the remaining dimensions, while making sure it satisfies the criterion that **the new** shape should be compatible with the original shape.

```
import numpy as np
a = np.array([[1, 2, 3, 4], [5, 6, 7, 8], [9, 10, 11, 12]])
print(a.shape) # Prints (3, 4)
# Reshaping with *just* (-1) leads to array flattening.
# Yields new shape as (12,), a rank 1 array which is compatible with original shape (3, 4)
print(a.reshape(-1)) # Prints [ 1 2 3 4 5 6 7 8 9 10 11 12]
# Note that np.reshape(-1) returns the same result as np.flatten()
# with the exception that np.flatten() returns a copy while reshape() returns a view of the original array.
# For more on np.flatten(), refer the section on "flatten" below.
# Transform a matrix to a row vector by reshaping with (1, -1), i.e., 1 row and 3*4 number of columns.
# Yields new shape as (1, 12), a rank 2 array which is compatible with original shape (3, 4)
print(a.reshape(1, -1)) # Prints [[ 1 2 3 4 5 6 7 8 9 10 11 12]]
# Transform a matrix to a column vector by reshaping with (-1, 1), i.e., 3*4 number of rows and 1 column.
# Yields new shape as (12, 1), a rank 2 array which is compatible with original shape (3, 4)
print(a.reshape(-1, 1)) # Prints [[ 1],
                       #
                                 [ 2],
                                 [3],
                                 [4],
                                 [5],
                                 [6],
                                 [7],
                                 [8],
                                 [ 9],
                                 [10],
                                 [11],
                                 [12]]
```

#### ▼ Flatten

• Return a **copy** of the array collapsed into one dimension.

```
import numpy as np
a = np.array([[1, 2, 3], [4, 5, 6]])
print(a.flatten()) # Prints [1, 2, 3, 4, 5, 6]
```

# ▼ Squeeze

• Remove single-dimensional entries from the shape of an array.

```
import numpy as np
a = np.array([[[0], [1], [2]]])

print(a.shape)  # Prints (1, 3, 1)
print(np.squeeze(a))  # Prints [0 1 2]
print(np.squeeze(a).shape) # Prints (3,)
```

# ▼ Copy

• Return an array copy of the given object.

```
a[0] == b[0] # Prints True
a[0] == c[0] # Prints False
```

• Note that np.copy() performs a shallow copy and will **not** copy object elements within arrays. This is mainly important for arrays containing Python objects.

## ▼ Transpose

• To transpose a 2D array (matrix), i.e., **swap rows and columns**, simply use the T attribute of an array object. Note that np.transpose() and <ndarray>.transpose() also yields the same result.

• With np.transpose(), you can not only transpose a matrix but also rearrange the axes of a multidimensional array in any order.

```
import numpy as np
a = np.ones((1, 2, 3))
```

```
print(a.shape) # Prints (1, 2, 3)
print(np.transpose(a, (1, 0, 2)).shape) # Prints (2, 1, 3)
```

# ▼ Element-wise sign

• Returns an element-wise sign of an array's elements.

### **▼** Sum

• Sum of an array's elements.

```
import numpy as np
a = np.array([[1, 2], [3, 4]])

# Compute sum of all elements
print(np.sum(a))  # Prints 10

# Compute sum of each column
print(np.sum(a, axis=0)) # Prints [4 6]

# Compute sum of each row
print(np.sum(a, axis=1)) # Prints [3 7]
```

# ▼ Average/Mean

• Recall that the mean is the sum of the elements divided by the length of the vector.

```
import numpy as np

a = np.array([[1, -1], [2, -2], [3, -3]]) # Define a 3x2 matrix. Chosen to be a matrix with 0 mean.

# Get the mean for the whole matrix
print(np.mean(a)) # Prints 0.0

# Get the mean for each column. Returns 2 elements.
print(a, axis=0) # Prints [ 2. -2.]

# Get the mean for each row. Returns 3 elements.
print(a, axis=1) # Prints [0. 0. 0.]
```

#### ▼ Product

• Return the product of array elements over a given axis.

```
import numpy as np
a = np.array([[1, 2], [3, 4]])
print(np.prod(a)) # Prints 24
```

### ▼ Max

• Return the maximum element of an array or maximum along an axis.

```
import numpy as np
a = np.array([[1, 2, 3], [4, 5, 6]])
print(np.max(a)) # Prints 6
```

#### ▼ Element-wise max

• Compare two compatible arrays and return their element-wise maximum. Here, 'compatible' means that one array can be broadcast to the other.

## ▼ Argmax

· Return the indices of the maximum values along an axis.

```
import numpy as np
a = np.array([[1, 2, 3], [4, 5, 6]])
print(np.argmax(a))  # Prints 5
print(np.argmax(a, axis=0)) # Prints [1 1 1]
print(np.argmax(a, axis=1)) # Prints [2 2]
```

• Note that in case of multiple occurrences of the maximum values, only the index corresponding to the first occurrence is returned.

### ▼ Argmin

Return the indices of the minimum values along an axis.

```
import numpy as np
a = np.array([[1, 2, 3], [4, 5, 6]])
print(np.argmin(a))  # Prints 0
print(np.argmin(a, axis=0)) # Prints [0 0 0]
print(np.argmin(a, axis=1)) # Prints [0 0]
```

• Note that in case of multiple occurrences of the minimum values, only the index corresponding to the first occurrence is returned.

#### ▼ Where

- Return elements chosen from x or y depending on condition.
- np.where() accepts three arguments: (condition, x, y). It first evaluates the condition argument -- if it returns True, it yields x, otherwise yields y.

```
import numpy as np
a = np.array([0, 1, 2, 3, 4, 5])
print(np.where(a < 3, a, 10*a)) # Prints [ 0 1 2 30 40 50]</pre>
```

#### ▼ Pad

- Pad an array.
- np.pad() accepts three arguments: array, pad\_width, mode='constant'.
  - o pad\_width specifies the number of values padded to the edges of each axis. It accepts both an int and a tuple.
    - (pad,) or simply a pad (as an int) is a shortcut for before = after = pad width for all axes.
    - ((before\_1, after\_1), ... (before\_N, after\_N)) specifies the padding widths for each axis.
    - ((before, after),) yields same before and after padding width for each axis.

- When mode is set to constant (which is default), an optional parameter constant\_values let's you specify the padding values for each axis, which has a default of Ø (i.e., zero padding). Rather than just an int, constant values accepts a tuple as well:
  - (constant,) or simply a constant (as an int) is a shortcut for before = after = constant for all axes. Default is 0.
  - ((before\_1, after\_1), ... (before\_N, after\_N)) specifies the unique pad constants for each axis.
  - ((before, after),) yields same before and after constants for each axis.

#### ▼ Ravel

- Return a contiguous flattened array.
- Note that np.ravel() returns a **view** of the array when the elements are contiguous in memory (just like <a href="np.reshape()">np.reshape()</a>). So modifying the result of np.ravel() would also modify the original array. However, np.ravel() returns a copy if, for e.g., the input array were made from slicing another array using a **non-unit** step size (e.g. a = x[::2]).

```
import numpy as np
a = np.array([[1, 2, 3], [4, 5, 6]])
print(np.ravel(a)) # Prints [1, 2, 3, 4, 5, 6]
```

• Note that np.ravel() is equivalent to np.reshape(-1).

```
import numpy as np
a = np.array([[1, 2, 3], [4, 5, 6]])
print(np.reshape(a, -1)) # Prints [1, 2, 3, 4, 5, 6])
```

#### ▼ Unravel Index

- Converts a "flat" index (i.e., an index into the flattened version of an array) into a tuple of coordinate arrays.
- Background:
  - $\circ$  Computer memory is addressed linearly. Each memory cell corresponds to a number. A block of memory can be addressed in terms of a base, which is the memory address of its first element, and the item index. For example, assuming the base address is 10,000:

```
item index 0 1 2 3
memory address 10,000 10,001 10,002 10,003
```

- To store multi-dimensional blocks, their geometry must somehow be made to fit into linear memory. In C and NumPy, this is done row-

- So, for example, in this 3-by-4 block the 2D index \\((1, 2)\\) would correspond to the linear index \\((6\\)) which is \\(1 \times 4
- `np.unravel\_index()` does the inverse. Given a linear index, it computes the corresponding coordinates. Since this depends on ' b

```
import numpy as np

# Passing an integer array whose elements are indices into the flattened version of an array
print(np.unravel_index([1, 2, 3], (4, 5)) # Prints (array([0, 0, 0]), array([1, 2, 3]))

# You're not limited to the 2-dimensional XY co-ordinate space
print(np.unravel_index(7, (1, 1, 7))) # Prints (0, 0, 6)
```

## Exponential

Calculate the exponential of all elements in the input array.

### ▼ Unique

• Find the unique elements of an array.

```
import numpy as np
a = np.array([[1, 1, 1], [2, 2, 2]])
print(np.unique(a)) # Prints [1 2]
```

#### ▼ Bincount

• Count number of occurrences of each value in a one-dimensional array of non-negative integers.

```
import numpy as np
a = np.array([1, 1, 1, 2, 2, 2])
print(np.bincount(a)) # Prints [0 3 3]
```

# ▼ Element-wise square

• Return the element-wise square of the input.

### ▼ Element-wise square root

• Return the element-wise non-negative square root of an array.

# ▼ Split

• Split an array into multiple sub-arrays.

```
import numpy as np
a = np.arange(8)
print(np.split(a, 2)) # Prints [array([0, 1, 2, 3]), array([4, 5, 6, 7])]
```

# ▼ Horizontal split

• Split an array into multiple sub-arrays horizontally (column-wise).

# ▼ Vertical split

• Split an array into multiple sub-arrays vertically (row-wise).

```
print(np.vsplit(a, 2)) # Prints [array([[0, 1]]), array([[2, 3]])]
```

### → Stack

• Join a sequence of arrays along a new axis. Note that by default, axis is set to 0 implying it joins arrays row-wise.

```
import numpy as np
a = np.array([1, 2, 3])
b = np.array([4, 5, 6])
print ((a,b))
                               # Prints (array([1, 2, 3]), array([4, 5, 6]))
                               # Prints [[1 2 3],
print(np.stack((a, b)))
                                         [4 5 6]]
# This is the same as above since axis is set to 0 by default
print(np.stack((a, b), axis=0)) # Prints [[1 2 3],
                                         [4 5 6]]
# np.vstack() matches the output of np.stack().
# Note that np.vstack() is discussed in more detail below.
print(np.vstack(a, b))
                                # Prints [[1 2 3],
                                         [4 5 6]]
# Joining arrays column-wise.
print(np.stack((a, b), axis=1)) # Prints [[1 4],
                                          [2 5],
                                         [3 6]]
# np.hstack() does *not* match the output of np.stack().
print(np.hstack((a, b)))
                             # Prints [1 2 3 4 5 6]
```

### ▼ Horizontal stack

- Stack arrays in sequence horizontally (column wise).
- Note that np.hstack() does not accept an axis argument.

```
import numpy as np
a = np.array([1, 2, 3])
b = np.array([4, 5, 6])
print(np.hstack((a, b))) # Prints [1 2 3 4 5 6]
```

#### ▼ Vertical stack

- Stack arrays in sequence vertically (row wise).
- Note that np.vstack() does not accept an axis argument.

### ▼ Concatenate

• Join a sequence of arrays along an existing axis.

```
import numpy as np
```

### ▼ Test any

- Test whether any array element along a given axis evaluates to True.
- Returns a single boolean unless axis is not None (which is the default).
- Note that not a number (NaN),  $\infty$  and  $-\infty$  all evaluate to True because these are not equal to 0.

```
import numpy as np
a = [[True, False], [True, True]]
print(np.any(a))
                                         # Prints True
a = [[True, False], [True, True]]
print(np.any(a, axis=0))
                                         # Prints [ True, True]
a = np.array([[1, 2], [3, 4]])
print(np.any(a))
                                         # Prints True
# A nifty use-case of np.any() is to select elements that satisfy
# atleast one condition from multiple given conditions
a = np.array([[1, 2], [3, 4]])
print(np.any([a > 1, a < 5], axis=0))
                                        # Prints [[ True True]
                                                   [ True True]]
print(a[np.any([a > 1, a < 5], axis=0)]) # Prints [1 2 3 4]
# If axis is None (default), np.any() yields a single boolean by performing
# a logical OR reduction over all the dimensions of the input array
print(np.any([a > 1, a < 5]))
                                         # Prints True
```

#### ▼ Test all

- Test whether all array elements along a given axis evaluate to True.
- Similar to np.any(), np.all() returns a single boolean unless axis is not None (which is the default).
- Again, similar to np.any(), note that not a number (NaN),  $\infty$  and  $-\infty$  all evaluate to True because these are not equal to 0.

```
import numpy as np
a = [[True, False], [True, True]]
print(np.all(a))
                                        # Prints True
a = [[True, False], [True, True]]
print(np.all(a, axis=0))
                                        # Prints [ True, False]
a = np.array([[1, 2], [3, 4]])
print(np.all(a))
                                        # Prints True
# A nifty use-case of np.all() is to select elements that satisfy
# all given conditions
a = np.array([[1, 2], [3, 4]])
print(np.all([a > 1, a < 5], axis=0))
                                        # Prints [[False True]
                                                  [ True Truell
print(a[np.all([a > 1, a < 5], axis=0)]) # Prints [2 3 4]
# Note that if only one condition is specified, np.any() and np.all()
# are equivalent, and have identical outputs
print(a[np.any([a > 1], axis=0)])
                                  # Prints [2 3 4]
print(a[np.all([a > 1], axis=0)])
                                  # Prints [2 3 4]
# If axis is None (default), np.all() yields a single boolean by performing
# a logical AND reduction over all the dimensions of the input array
print(np.all([a > 1, a < 5]))
                                        # Prints False
```

### References and credits

- Parts of this tutorial were originally contributed by <u>Justin Johnson</u>.
- Stanford CS231n Python/NumPy Tutorial served as a major inspiration for this tutorial.
- NumPy documentation: Broadcasting
- What is an intuitive explanation of np.unravel\_index?
- When should I use hstack/vstack vs. append vs. concatenate vs. column\_stack?
- What is the difference between NumPy's array() and asarray() functions?
- What does -1 mean in NumPy reshape?
- Find the most frequent number in a NumPy vector
- NumPy: From ND to 1D arrays
- <u>Difference between functions generating random numbers in NumPy</u>
- How do I select elements of an array given condition?

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