Numpy Handbook

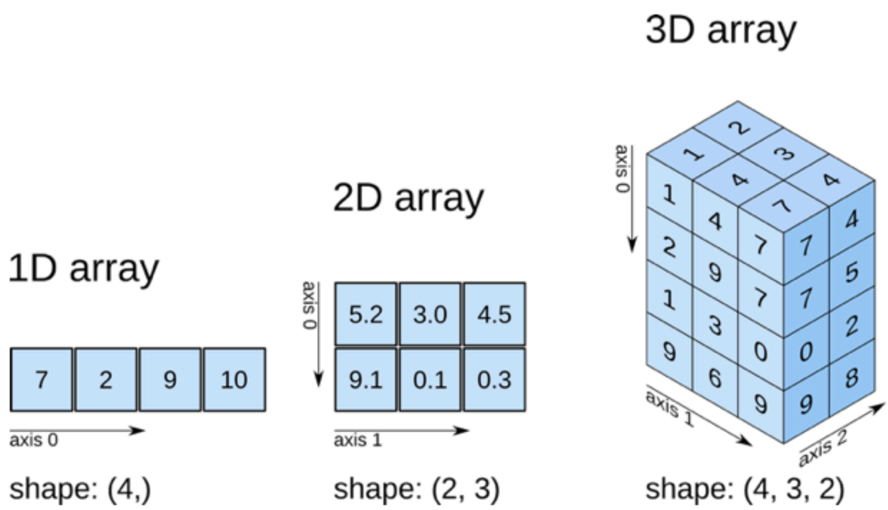
By Patrick Loeber - Available at python-engineer.com

Learn NumPy with this Handbook! It covers code examples for all essential functions and some tricks and useful methods. NumPy is the core library for scientific computing in Python. It is essential for any **data science** or **machine learning** algorithms.

Outline

1. NumPy Introduction

NumPy is the **core library for scientific computing** in Python. The central object in the NumPy library is the NumPy array. The NumPy array is a **high-performance multidimensional array object**, which is designed specifically to perform math operations, **linear algebra**, and probability calculations. Using a NumPy array is usually a lot faster and needs less code than using a Python list. A huge part of the NumPy library consists of C code with the Python API serving as a wrapper around these C functions. This is one of the reasons why NumPy is so fast.



Most of the popular Machine Learning, Deep Learning, and Data Science libraries use NumPy under the hood:

- Scikit-learn
- Matplotlib
- Pandas

Different use cases and operations that can be achieved easily with NumPy:

- Dot product/inner product
- Matrix multiplication
- Element wise matrix product
- Solving linear systems
- Inverse
- Determinant
- Choose random numbers (e.g. Gaussian/Uniform)
- Working with images represented as array
- ... and many more

2. Installation and Array Basics

Installation with **pip** or **Anaconda**:

```
$ pip install numpy
or
$ conda install numpy
```

Import numpy:

```
import numpy as np
# check verion
np.__version__
# --> 1.19.1
```

Central object is the array:

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

a # [1 2 3 4 5]
a.shape # shape of the array: (5,)
a.dtype # type of the elements: int32
a.ndim # number of dimensions: 1
a.size # total number of elements: 5
a.itemsize # the size in bytes of each element: 4
```

Essential methods:

```
a = np.array([1,2,3])
# access and change elements
print(a[0]) # 1
a[0] = 5
print(a) # [5 2 3]

# elementwise math operations
b = a * np.array([2,0,2])
print(b) # [10 0 6]
print(a.sum()) # 10
```

3. Array vs List

```
l = [1,2,3]
a = np.array([1,2,3]) # create an array from a list
print(l) # [1, 2, 3]
print(a) # [1 2 3]

# adding new item
l.append(4)
#a.append(4) error: size of array is fixed

# there are ways to add items, but this essentially creates new arrays
l2 = l + [5]
print(l2) # [1, 2, 3, 4, 5]

a2 = a + np.array([4])
print(a2) # this is called broadcasting, adds 4 to each element
# -> [5 6 7]

# vector addidion (this is technically correct compared to broadcasting)
a3 = a + np.array([4,4,4])
print(a3) # [5 6 7]

#a3 = a + np.array([4,5]) # error, can't add vectors of different sizes

# multiplication
l2 = 2 * l # list l repeated 2 times, same a l+l
print(l2)
# -> [1, 2, 3, 4, 1, 2, 3, 4]

a3 = 2 * a # multiplication for each element

print(a3)
# -> [2 4 6]

# modify each item in the list
l2 = []
for i in l:
  l2.append(i**2)
print(l2) # [1, 4, 9, 16]

# or list comprehension
l2 = [i**2 for i in l]
print(l2) # [1, 4, 9, 16]

a2 = a**2 # -> squares each element!
```

```
print(a2) # [1 4 9]

# Note: function applied to array usually operates element wise
a2 = np.sqrt(a) # np.exp(a), np.tanh(a)
print(a2) # [1. 1.41421356 1.73205081]
a2 = np.log(a)
print(a2) # [0. 0.69314718 1.09861229]
```

4. Dot Product

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

# sum of the products of the corresponding entries
# multiply each corresponding elements and then take the sum

# cumbersome way for lists
dot = 0
for i in range(len(a)):
  dot += a[i] * b[i]
print(dot) # 11

# easy with numpy :)
dot = np.dot(a,b)
print(dot) # 11

# step by step manually
c = a * b
print(c) # [3 8]
d = np.sum(c)
print(d) # 11

# most of these functions are also instance methods
dot = a.dot(b)
print(dot) # 11
dot = (a*b).sum()
print(dot) # 11

# in newer versions
dot = a @ b
print(dot) # 11
```

5. Speed Test Array vs List

```
from timeit import default_timer as timer

a = np.random.randn(1000)
b = np.random.randn(1000)

A = list(a)
B = list(b)

T = 1000

def dot1():
  dot = 0
  for i in range(len(A)):
    dot += A[i]*B[i]
  return dot

def dot2():
  return np.dot(a,b)

start = timer()
for t in range(T):
  dot1()
end = timer()
t1 = end-start

start = timer()
for t in range(T):
  dot2()
end = timer()
t2 = end-start

print('Time with lists:', t1) # -> 0.19371
print('Time with array:', t2) # -> 0.00112
print('Ratio', t1/t2)         # -> 172.332 times faster
```

6. Multidimensional (nd) Arrays

```
# (matrix class exists but not recommended to use)
a = np.array([[1,2], [3,4]])
print(a)
```

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

print(a.shape) # (2, 2)

# Access elements
# row first, then columns

print(a[0]) # [1 2]
print(a[0][0]) # 1
# or
print(a[0,0]) # 1

# slicing
print(a[:,0]) # all rows in col 0:    [1 3]
print(a[0,:]) # all columns in row 0: [1 2]

# transpose
a.T

# matrix multiplication
b = np.array([[3, 4], [5,6]])
c = a.dot(b)

d = a * b # elementwise multiplication

# inner dimensions must match!
b = np.array([[1,2,3], [4,5,6]])
c = a.dot(b.T)

# determinant
c = np.linalg.det(a)

# inverse
c = np.linalg.inv(a)

# diag
c = np.diag(a)
print(c) # [1 4]

# diag on a vector returns diagonal matrix (overloaded function)
c = np.diag([1,4])
print(c)
# [[1 0]
#  [0 4]]
```

7. Indexing, Slicing, And Boolean Indexing

Indexing and Slicing:

```
# 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:
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]]

# Integer array indexing
b = a[0,1]
print(b) # 2

# Slicing
row0 = a[0,:]
print(row0) # [1 2 3 4]

col0 = a[:, 0]
print(col0) # [1 5 9]

slice_a = a[0:2,1:3]
print(slice_a)
# [[2 3]
#  [6 7]]

# indexing starting from the end: -1, -2 etc...
last = a[-1,-1]
print(last) # 12
```

Boolean indexing:

```
# Boolean indexing:
a = np.array([[1,2], [3, 4], [5, 6]])
print(a)
# [[1 2]
#  [3 4]
#  [5 6]]

# same shape with True or False for the condition
bool_idx = a > 2
print(bool_idx)
```

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

# note: this will be a rank 1 array!
print(a[bool_idx]) # [3 4 5 6]

# We can do all of the above in a single concise statement:
print(a[a > 2]) # [3 4 5 6]

# np.where(): same size with modified values
b = np.where(a>2, a, -1)
print(b)
# [[-1 -1]
#  [ 3 4]
#  [ 5 6]]

# fancy indexing: access multiple indices at once
a = np.array([10,19,30,41,50,61])

b = a[[1,3,5]]
print(b) # [19 41 61]

# compute indices where condition is True
even = np.argwhere(a%2==0).flatten()
print(even) # [0 2 4]

a_even = a[even]
print(a_even) # [10 30 50]
```

8. Reshaping

```
a = np.arange(1, 7)
print(a) # [1 2 3 4 5 6]

b = a.reshape((2, 3)) # error if shape cannot be used
print(b)
# [[1 2 3]
#  [4 5 6]]

c = a.reshape((3, 2)) # 3 rows, 2 columns
print(c)
# [[1 2]
#  [3 4]
#  [5 6]]
```

```
# newaxis is used to create a new axis in the data
# needed when model require the data to be shaped in a certain manner
print(a.shape) # (6,)

d = a[np.newaxis, :]
print(d) # [[1 2 3 4 5 6]]
print(d.shape) # (1, 6)

e = a[:, np.newaxis]
print(e)
# [[1]
#  [2]
#  [3]
#  [4]
#  [5]
#  [6]]

print(e.shape) # (6, 1)
```

9. Concatenation

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

# combine into 1d
c = np.concatenate((a, b), axis=None)
print(c) # [1 2 3 4 5 6]

# add new row
d = np.concatenate((a, b), axis=0)
print(d)
# [[1 2]
#  [3 4]
#  [5 6]]

# add new column: note that we have to transpose b!
e = np.concatenate((a, b.T), axis=1)
print(e)
# [[1 2 5]
#  [3 4 6]]

# hstack: Stack arrays in sequence horizontally (column wise). needs a tuple
a = np.array([1,2,3,4])
b = np.array([5,6,7,8])
```

```
c = np.hstack((a,b))
print(c) # [1 2 3 4 5 6 7 8]

a = np.array([[1,2], [3,4]])
b = np.array([[5,6], [7,8]])
c = np.hstack((a,b))
print(c)
# [[1 2 5 6]
#  [3 4 7 8]]

# vstack: Stack arrays in sequence vertically (row wise). needs a tuple
a = np.array([1,2,3,4])
b = np.array([5,6,7,8])
c = np.vstack((a,b))
print(c)
# [[1 2 3 4]
#  [5 6 7 8]]

a = np.array([[1,2], [3,4]])
b = np.array([[5,6], [7,8]])
c = np.vstack((a,b))
print(c)
# [[1 2]
#  [3 4]
#  [5 6]
#  [7 8]]
```

10. 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.

```
x = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
y = np.array([1, 0, 1])
z = x + y # Add v to each row of x using broadcasting
print(z)
# [[ 2 2 4]
#  [ 5 5 7]
#  [ 8 8 10]
#  [11 11 13]]
```

11. Functions and Axis

```
a = np.array([[7,8,9,10,11,12,13], [17,18,19,20,21,22,23]])

print(a.sum())          # default=None-> 210
print(a.sum(axis=None)) # overall sum -> 210

print(a.sum(axis=0)) # along the rows -> 1 sum entry for each column
# -> [24 26 28 30 32 34 36]

print(a.sum(axis=1)) # along the columns -> 1 sum entry for each row
# -> [ 70 140]

print(a.mean())          # default=None-> 15.0
print(a.mean(axis=None)) # overall mean -> 15.0

print(a.mean(axis=0)) # along the rows -> 1 mean entry for each column
# -> [12. 13. 14. 15. 16. 17. 18.]

print(a.mean(axis=1)) # along the columns -> 1 mean entry for each row
# -> [10. 20.]

# some more: std, var, min, max
```

12. Datatypes

[Overview of all datatypes]

```
# Let numpy choose the datatype
x = np.array([1, 2])
print(x.dtype) # int32

# Let numpy choose the datatype
x = np.array([1.0, 2.0])
print(x.dtype) # float64

# Force a particular datatype, how many bits (how precise)
x = np.array([1, 2], dtype=np.int64) # 8 bytes
print(x.dtype) # int64

x = np.array([1, 2], dtype=np.float32) # 4 bytes
print(x.dtype) # float32
```

13. Copying

```
a = np.array([1,2,3])
b = a # only copies reference!
b[0] = 42
print(a) # [42 2 3]

a = np.array([1,2,3])
b = a.copy() # actual copy!
b[0] = 42
print(a) # [1 2 3]
```

14. Generating Arrays

```
# zeros
a = np.zeros((2,3)) # size as tuple
# [[0. 0. 0.]
#  [0. 0. 0.]]

# ones
b = np.ones((2,3))
# [[1. 1. 1.]
#  [1. 1. 1.]]

# specific value
c = np.full((3,3),5.0)
# [[5. 5. 5.]
#  [5. 5. 5.]
#  [5. 5. 5.]]

# identity
d = np.eye(3) #3x3
# [[1. 0. 0.]
#  [0. 1. 0.]
#  [0. 0. 1.]]

# arange
e = np.arange(10)
# [0 1 2 3 4 5 6 7 8 9]

# linspace
f = np.linspace(0, 10, 5)
```

```
# [ 0. 2.5 5. 7.5 10. ]
```

15. Random Numbers

```
a = np.random.random((3,2)) # uniform 0-1 distribution
# [[0.06121857 0.10180167]
#  [0.83321726 0.54906613]
#  [0.94170273 0.19447411]]

b = np.random.randn(3,2) # normal/Gaussian distribution, mean 0 and unit
variance
# no tuple as shape here! each dimension one argument
# [[ 0.56759123 -0.65068333]
#  [ 0.83445762 -0.36436185]
#  [ 1.27150812 -0.32906051]]

c = np.random.randn(10000)
print(c.mean(), c.var(), c.std())
# -0.0014 0.9933 0.9966

d = np.random.randn(10, 3)
print(d.mean()) # mean of whole array: -0.1076827228882305

# random integer, low,high,size; high is exclusive
e = np.random.randint(3,10,size=(3,3)) # if we only pass one parameter, then
from 0-x
print(e)
# [[6 8 4]
#  [3 6 3]
#  [4 7 8]]

# with integer is between 0 up to integer exclusive
f = np.random.choice(7, size=10)
# [2 0 4 5 1 3 4 0 0 6]

# with an array it draws random values from this array
g = np.random.choice([1,2,3,4], size=8)
# [4 2 1 3 4 1 4 1]
```

16. Linear Algebra (Eigenvalues / Solving Linear Systems)

Eigenvalues

```
a = np.array([[1,2], [3,4]])
eigenvalues, eigenvectors = np.linalg.eig(a)
# Note: use eigh if your matrix is symmetric (faster)

print(eigenvalues)
# [-0.37228132 5.37228132]

print(eigenvectors) # column vectors
# [[-0.82456484 -0.41597356]
#  [ 0.56576746 -0.90937671]]

print(eigenvectors[:,0]) # column 0 corresponding to eigenvalue[0]
# [-0.82456484 0.56576746]

# verify: e-vec * e-val = A * e-vec
d = eigenvectors[:,0] * eigenvalues[0]
e = a @ eigenvectors[:, 0]

print(d, e) # [ 0.30697009 -0.21062466] [ 0.30697009 -0.21062466]
# looks the same, but:
print(d == e) # [ True False] -> numerical issues

# correct way to compare matrix
print(np.allclose(d,e)) # True
```

Solving Linear Systems

```
#     x1 + x2    = 2200
# 1.5 x1 + 4 x2 = 5050
# -> 2 equations and 2 unknowns

A = np.array([[1, 1], [1.5, 4]])
b = np.array([2200,5050])

# Ax = b <=> x = A-1 b

# But: inverse is slow and less accurate
x = np.linalg.inv(A).dot(b) # not recommended
print(x) # [1500. 700.]
```

```python
# instead use:
x = np.linalg.solve(A,b) # good
print(x) # [1500. 700.]
```

17. Loading CSV files

```python
# 1) load with np.loadtxt()
# skiprows=1, ...
data = np.loadtxt('my_file.csv', delimiter=",",dtype=np.float32)
print(data.shape, data.dtype)

# 2) load with np.genfromtxt()
# similar but slightly more configuration parameters
# skip_header=0, missing_values="---", filling_values=0.0, ...
data = np.genfromtxt('my_file.csv', delimiter=",", dtype=np.float32)
print(data.shape)
```