Data Science - Wes McKinney: Chapter 4: NumPy Basics: Arrays and Vectorized Computation

Created by Travis Oliphant (2005). Importance of NumPy:

- NumPy internally stores data in a contiguous block of memory, independent of other built-in Python objects. NumPy's library of algorithms written in the C language can operate on this memory without any type checking or other overhead. NumPy arrays also use much less memory than built-in Python sequences.
- 2. NumPy operations perform complex computations on entire arrays without the need for Python for loops, which can be slow for large sequences. NumPy is faster than regular Python code because its C-based algorithms avoid overhead present with regular interpreted Python code.

4.1 The NumPy ndarray: A Multidimensional Array Object

ndarray: N-dimensional array.

It would be possible to put from numpy import * in your code to avoid having to write np., but I advise against making a habit of this. The numpy namespace is large and contains a number of functions whose names conflict with built-in Python functions (like min and max). Following standard conventions like these is almost always a good idea.

```
In [6]: print('shape:', data.shape, '\t dtype:', data.dtype)
shape: (2, 3) dtype: float64
```

Creating ndarrays

```
In [7]: data1 = [6, 7.5, 8, 0, 1]
        arr1 = np.array(data1)
        data2 = [[1, 2, 3, 4], [5, 6, 7, 8]]
        arr2 = np.array(data2)
        display(arr1, arr2)
        print(f'ndim: {arr1.ndim},\t shape: {arr1.shape},\t dtype: {arr1.dtype}')
        print(f'ndim: {arr2.ndim},\t shape: {arr2.shape},\t dtype: {arr2.dtype}')
        array([6., 7.5, 8., 0., 1.])
        array([[1, 2, 3, 4],
               [5, 6, 7, 8]])
                         shape: (5,),
                                         dtype: float64
        ndim: 1,
        ndim: 2,
                         shape: (2, 4), dtype: int32
In [8]: display(np.zeros(10), np.zeros((3,5)))
        display(np.empty((2,3,4)))
        display(np.arange(5))
        array([0., 0., 0., 0., 0., 0., 0., 0., 0., 0.])
        array([[0., 0., 0., 0., 0.],
               [0., 0., 0., 0., 0.]
               [0., 0., 0., 0., 0.]
        array([[[3.56043053e-307, 1.60219306e-306, 7.56571288e-307,
                 1.89146896e-307],
                [1.37961302e-306, 1.05699242e-307, 8.01097889e-307,
                 1.78020169e-306],
                [7.56601165e-307, 1.02359984e-306, 1.33510679e-306,
                 2.22522597e-306]],
               [[1.33511018e-306, 6.23057689e-307, 1.33511290e-306,
                 1.78019082e-306],
                [8.45559303e-307, 8.06613465e-308, 6.89810244e-307,
                 1.22387550e-307],
                [2.22522596e-306, 8.34423917e-308, 9.79107193e-307,
                 3.33509775e-317]])
        array([0, 1, 2, 3, 4])
```

To create a higher dimensional array, pass a tuple for the shape. It's not safe to assume that numpy.empty will return an array of all zeros. This function returns uninitialized memory and thus may contain nonzero "garbage" values.

Table 4-1. Some important NumPy array creation functions

- 1. array: Convert input data (list, tuple, array, or other sequence type) to an ndarray either by inferring a data type or explicitly specifying a data type; copies the input data by default
- 2. asarray: Convert input to ndarray, but do not copy if the input is already an ndarray
- 3. arange: Like the built-in range but returns an ndarray instead of a list
- 4. ones, ones_like: Produce an array of all 1s with the given shape and data type; ones_like takes another array and produces a ones array of the same shape and data type
- 5. zeros, zeros_like: Like ones and ones_like but producing arrays of 0s instead
- 6. empty, empty_like: Create new arrays by allocating new memory, but do not populate with any values like ones and zeros
- 7. full, full_like: Produce an array of the given shape and data type with all values set to the indicated "fill value"; full_like takes another array and produces a filled array of the same shape and data type
- 8. eye, identity: Create a square $N \times N$ identity matrix (1s on the diagonal and 0s elsewhere)

Data Types for ndarrays

```
In [9]: arr1 = np.array([1, 2, 3], dtype=np.float64)
arr2 = np.array([1, 2, 3], dtype=np.int32)
display(arr1.dtype, arr2.dtype)

dtype('float64')
dtype('int32')
```

Table 4-2. NumPy data types. page: 89

```
In [10]: arr = np.array([1, 2, 3, 4, 5])
         display(arr, arr.dtype)
         float_arr = arr.astype(np.float64)
         display(float_arr, float_arr.dtype)
         arr = np.array([3.7, -1.2, -2.6, 0.5, 12.9, 10.1])
         display(arr, arr.dtype)
         display(arr.astype(np.int32))
         numeric_strings = np.array(["1.25", "-9.6", "42"], dtype=np.string_)
         display(numeric_strings, numeric_strings.dtype)
         display(numeric_strings.astype(complex))
         array([1, 2, 3, 4, 5])
         dtype('int32')
         array([1., 2., 3., 4., 5.])
         dtype('float64')
         array([ 3.7, -1.2, -2.6, 0.5, 12.9, 10.1])
         dtype('float64')
         array([ 3, -1, -2, 0, 12, 10])
         array([b'1.25', b'-9.6', b'42'], dtype='|S4')
         dtype('S4')
         array([ 1.25+0.j, -9.6 +0.j, 42. +0.j])
```

Be cautious when using the numpy.string_type, as string data in NumPy is fixed size and may truncate input without warning. pandas has more intuitive out-of-the-box behavior on non-numeric data. If casting were to fail for some reason (like a string that cannot be converted to float64), a ValueError will be raised.

Calling astype always creates a new array (a copy of the data), even if the new data type is the same as the old data type.

```
In [11]: int_array = np.arange(10)
    calibers = np.array([.22, .270, .357, .380, .44, .50], dtype=np.float64)
    display(int_array.astype(calibers.dtype))

# Short-hands
    zeros_uint32 = np.zeros(8, dtype="u4")
    display(zeros_uint32)

array([0., 1., 2., 3., 4., 5., 6., 7., 8., 9.])
    array([0, 0, 0, 0, 0, 0, 0], dtype=uint32)
```

Arithmetic with NumPy Arrays:

Arrays are important because they enable you to express batch operations on data without writing any for loops. NumPy users call this **vectorization**. Any arithmetic operations between equal-size arrays apply the operation element-wise.

Basic Indexing and Slicing:

```
In [13]: arr = np.arange(10)
    display(arr, arr[5])
    arr_slice = arr[5:8]
    display(arr_slice)
    arr_slice[:]=100
    display(arr_slice, arr)

array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
    5
    array([5, 6, 7])
    array([100, 100, 100])
    array([ 0,  1,  2,  3,  4, 100, 100, 100,  8,  9])
```

An important first distinction from Python's built-in lists is that array slices are views on the original array. This means that the data is not copied, and any modifications to the view will be reflected in the source array.

If you want a copy of a slice of an ndarray instead of a view, you will need to explicitly copy the array—for example, arr[5:8].copy(). As you will see, pandas works this way, too.

2D: Think, axis 0 as the "rows" of the array and axis 1 as the "columns".

```
In [15]:
         arr3d = np.array([[[1, 2, 3], [4, 5, 6]], [[7, 8, 9], [10, 11, 12]]])
         display(arr3d, arr3d.shape, arr3d[1,1,0])
         old_values = arr3d[0].copy()
         arr3d[0] = 42
         display(arr3d, old_values)
         arr3d[0] = old_values
         display(arr3d)
         array([[[ 1, 2, 3],
                 [4, 5, 6]],
                [[ 7, 8, 9],
                 [10, 11, 12]]])
         (2, 2, 3)
         10
         array([[[42, 42, 42],
                 [42, 42, 42]],
                [[ 7, 8, 9],
                 [10, 11, 12]])
         array([[1, 2, 3],
                [4, 5, 6]])
         array([[[ 1, 2, 3],
                 [4, 5, 6]],
                [[ 7, 8, 9], [10, 11, 12]]])
```

This multidimensional indexing syntax for NumPy arrays will not work with regular Python objects, such as lists of lists.

Indexing with slices: Pass multiple slices just like you can pass multiple indexes.

See Figure 4-2. Two-dimensional array slicing. page: 97

Boolean Indexing:

The ~ operator can be useful when you want to invert a Boolean array.

To select two of the three names to combine multiple Boolean conditions, use Boolean arithmetic operators like & (and) and | (or). The Python keywords and and or do not work with Boolean arrays. Use & (and) and | (or) instead.

```
In [17]: # Suppose each name corresponds to a row in the data array
         names = np.array(["Bob", "Joe", "Will", "Bob", "Will", "Joe", "Joe"])
         data = np.array([[4, 7], [0, 2], [-5, 6], [0, 0], [1, 2], [-12, -4], [3, 4]])
         display(names, data)
         display(names=='Joe', data[names=='Joe'])
         display('slicing', data[names=='Joe', 1], data[names=='Joe', 1:])
         display('invert conditions', names!='Joe', ~(names=='Joe'))
         cond = names=='Joe'
         display(data[~cond])
         mask = (names=='Bob')|(names=='Will')
         display('& (and) and | (or)', mask, data[mask])
         data[data<0] = 0</pre>
         display(data)
         data[(names!='Joe') & ~(names=='Bob')] = 10
         display(data)
         array(['Bob', 'Joe', 'Will', 'Bob', 'Will', 'Joe', 'Joe'], dtype='<U4')</pre>
         array([[ 4,
                        7],
                [ 0,
                        2],
                [ -5,
                        6],
                [ 0,
                        0],
                        2],
                [ 1,
                       -4],
                [-12,
                [ 3,
                        4]])
         array([False, True, False, False, False, True, True])
         array([[ 0,
                        2],
                [-12,
                       -4],
                [ 3,
                        4]])
         'slicing'
         array([ 2, -4, 4])
         array([[ 2],
                [-4],
                [ 4]])
         'invert conditions'
         array([ True, False, True, True, True, False, False])
         array([ True, False, True, True, True, False, False])
         array([[ 4, 7],
                [-5, 6],
                [0, 0],
                [ 1, 2]])
         '& (and) and | (or)'
         array([ True, False, True, True, True, False, False])
         array([[ 4, 7],
                [-5, 6],
                [0, 0],
                [ 1, 2]])
         array([[4, 7],
                [0, 2],
                [0, 6],
                [0, 0],
                [1, 2],
                [0, 0],
                [3, 4]])
```

Selecting data from an array by Boolean indexing and assigning the result to a new variable always creates a copy of the data, even if the returned array is unchanged.

Operations on two-dimensional data are convenient to do with pandas.

Fancy Indexing

To select a subset of the rows in a particular order, you can simply pass a list or ndarray of integers specifying the desired order. Passing multiple index arrays does something slightly different; it selects a one-dimensional array of elements corresponding to each tuple of indices.

Fancy indexing, unlike slicing, always copies the data into a new array when assigning the result to a new variable.

```
In [18]: arr = np.zeros((8, 4))
            for i in range(8):
                 arr[i] = i
            # for i in range(4):
                  arr[:,i] = i
            display(arr)
            display(arr[[4,3,0,7]], arr[[-2, -4, -7]])
            array([[0., 0., 0., 0.],
                     [1., 1., 1., 1.],
                    [2., 2., 2., 2.],
[3., 3., 3., 3.],
[4., 4., 4., 4.],
[5., 5., 5., 5.],
                     [6., 6., 6., 6.],
                     [7., 7., 7., 7.]])
            array([[4., 4., 4., 4.],
                     [3., 3., 3., 3.],
                    [0., 0., 0., 0.],
[7., 7., 7., 7.]])
            array([[6., 6., 6., 6.],
                     [4., 4., 4., 4.],
[1., 1., 1., 1.]])
```

```
In [19]: | arr = np.arange(32).reshape((8, 4))
         display(arr, arr[[1, 5, 7, 2], [0, 3, 1, 2]])
         print('Here the elements (1, 0), (5, 3), (7, 1), and (2, 2) were selected.')
         display(arr[[1, 5, 7, 2]][:, [0, 3, 1, 2]])
         print('rectangular region formed by selecting a subset of the matrix's rows and columns.')
         arr[[1, 5, 7, 2], [0, 3, 1, 2]] = 0
         display(arr)
         array([[ 0, 1, 2, 3],
                 [ 4, 5, 6, 7],
[ 8, 9, 10, 11],
                 [12, 13, 14, 15],
                 [16, 17, 18, 19],
                 [20, 21, 22, 23],
                 [24, 25, 26, 27],
                 [28, 29, 30, 31]])
         array([ 4, 23, 29, 10])
         Here the elements (1, 0), (5, 3), (7, 1), and (2, 2) were selected.
         array([[ 4, 7, 5, 6],
                 [20, 23, 21, 22],
                 [28, 31, 29, 30],
                 [ 8, 11, 9, 10]])
         rectangular region formed by selecting a subset of the matrix's rows and columns.
         array([[ 0, 1, 2, 3],
                 [ 0, 5, 6, 7],
[ 8, 9, 0, 11],
                 [12, 13, 14, 15],
                 [16, 17, 18, 19],
                 [20, 21, 22, 0],
                 [24, 25, 26, 27],
                 [28, 0, 30, 31]])
```

Transposing Arrays and Swapping Axes

Simple transposing with .T is a special case of swapping axes. ndarray has the method swapaxes, which takes a pair of axis numbers and switches the indicated axes to rearrange the data.

swapaxes similarly returns a view on the data without making a copy.

```
In [20]: | arr = np.arange(15).reshape((3, 5))
         display(arr, arr.T)
         arr = np.array([[0, 1, 0], [1, 2, -2], [6, 3, 2], [-1, 0, -1], [1, 0, 1]])
         display('matrix multiplication', np.dot(arr.T, arr), arr.T@arr)
         print('The @ infix operator is another way to do matrix multiplication.')
         display('swapaxes', arr, arr.swapaxes(0,1))
         array([[ 0, 1, 2, 3, 4],
                [5, 6, 7, 8, 9],
                [10, 11, 12, 13, 14]])
         array([[ 0, 5, 10],
                [ 1, 6, 11],
                [ 2, 7, 12],
                [3, 8, 13],
                [4, 9, 14]])
         'matrix multiplication'
         array([[39, 20, 12],
                [20, 14, 2],
                [12, 2, 10]])
         array([[39, 20, 12],
                [20, 14, 2],
                [12, 2, 10]])
         The @ infix operator is another way to do matrix multiplication.
         'swapaxes'
         array([[ 0, 1, 0],
               [ 1,
                     2, -2],
                [6, 3, 2],
                [-1, 0, -1],
                [ 1, 0, 1]])
         array([[ 0, 1, 6, -1,
                                1],
                [ 1, 2, 3, 0,
                                 0],
                [0, -2, 2, -1,
                                1]])
```

4.2 Pseudorandom Number Generation

The numpy random module supplements the built-in Python random module with functions for efficiently generating whole arrays of sample values from many kinds of probability distributions.

These random numbers are not truly random (rather, pseudorandom) but instead are generated by a configurable random number generator that determines determin- istically what values are created. Functions like numpy.random.standard normal use the numpy.random module's default random number generator.

The seed argument is what determines the initial state of the generator, and the state changes each time the rng object is used to generate data. The generator object rng is also isolated from other code which might use the numpy.random module.

Table 4-3. NumPy random number generator methods

- 1. permutation: Return a random permutation of a sequence, or return a permuted range
- 2. shuffle: Randomly permute a sequence in place
- 3. uniform: Draw samples from a uniform distribution
- 4. integers: Draw random integers from a given low-to-high range
- 5. standard normal: Draw samples from a normal distribution with mean 0 and standard deviation 1
- 6. binomial: Draw samples from a binomial distribution
- 7. normal: Draw samples from a normal (Gaussian) distribution
- 8. beta: Draw samples from a beta distribution
- 9. chisquare: Draw samples from a chi-square distribution
- 10. gamma: Draw samples from a gamma distribution
- 11. uniform: Draw samples from a uniform [0, 1) distribution

4.3 Universal Functions: Fast Element-Wise Array Functions

A universal function, or ufunc, is a function that performs element-wise operations on data in ndarrays. You can think of them as fast vectorized wrappers for simple functions that take one or more scalar values and produce one or more scalar results.

unary ufunc: takes one array as input; binary ufunc: takes 2 arrays as input.

```
In [26]: arr = np.arange(10)
         display(arr, 'ufunc', np.sqrt(arr), np.exp(arr))
         x, y = rng.standard normal(8), rng.standard normal(8)
         display(x, y)
         display(np.maximum(x,y))
         print('numpy.maximum computes the element-wise maximum of the elements in x and y')
         print('''numpy.modf is a vectorized version of the built-in Python math.modf,
         it returns the fractional and integral parts of a floating-point array''')
         arr = rng.standard normal(7) * 5
         remainder, whole part = np.modf(arr)
         display(remainder, whole_part)
         print('''optional out arguement -
             assign results into an existing array rather than create a new one''')
         display(arr)
         out1 = np.zeros_like(arr)
         np.add(arr, 1)
         np.add(arr, 2, out=out1)
         display(out1)
         array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
         'ufunc'
                          , 1.
                                      , 1.41421356, 1.73205081, 2.
         array([0.
                2.23606798, 2.44948974, 2.64575131, 2.82842712, 3.
         array([1.00000000e+00, 2.71828183e+00, 7.38905610e+00, 2.00855369e+01,
                5.45981500e+01, 1.48413159e+02, 4.03428793e+02, 1.09663316e+03,
                2.98095799e+03, 8.10308393e+03])
         array([-1.3677927 , 0.6488928 , 0.36105811, -1.95286306, 2.34740965,
                 0.96849691, -0.75938718, 0.90219827])
         array([-0.46695317, -0.06068952, 0.78884434, -1.25666813, 0.57585751,
                 1.39897899, 1.32229806, -0.29969852])
         array([-0.46695317, 0.6488928, 0.78884434, -1.25666813, 2.34740965,
                 1.39897899, 1.32229806, 0.90219827])
         numpy.maximum computes the element-wise maximum of the elements in \boldsymbol{x} and \boldsymbol{y}
         numpy.modf is a vectorized version of the built-in Python math.modf,
         it returns the fractional and integral parts of a floating-point array
         array([ 0.51459671, -0.10791367, -0.7909463 , 0.24741966, -0.71800536,
                -0.40843795, 0.62369966])
         array([ 4., -8., -0., 2., -6., -0., 8.])
         optional out arguement -
             assign results into an existing array rather than create a new one
         array([ 4.51459671, -8.10791367, -0.7909463 , 2.24741966, -6.71800536,
                -0.40843795, 8.62369966])
         array([ 6.51459671, -6.10791367, 1.2090537, 4.24741966, -4.71800536,
                 1.59156205, 10.62369966])
         Table 4-4. Some unary universal functions
```

page - 107

Table 4-5. Some binary universal functions

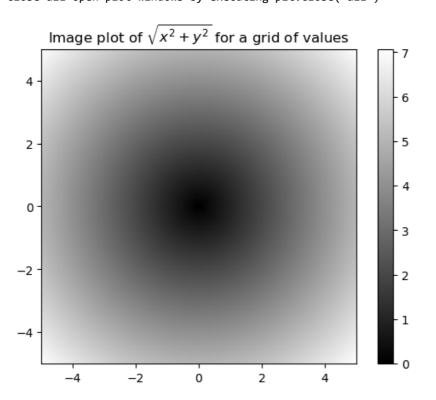
page - 107

4.4 Array-Oriented Programming with Arrays

Practice of replacing explicit loops with array expressions is referred to by some people as **vectorization** (faster than their pure Python equivalents).

```
In [27]: points = np.arange(-5, 5, 0.01) # 100 equally spaced points
          xs, ys = np.meshgrid(points, points)
          display(ys)
          z = np.sqrt(xs**2 + ys**2)
          display(z)
          import matplotlib.pyplot as plt
          plt.imshow(z, cmap=plt.cm.gray, extent=[-5,5,-5,5])
          plt.colorbar()
          plt.title("Image plot of \sqrt{x^2 + y^2} for a grid of values")
          # plt.close('all')
          print('close all open plot windows by executing plt.close("all")')
          array([[-5. , -5. , -5. , ..., -5. , -5. , -5. ],
                 [-4.99, -4.99, -4.99, ..., -4.99, -4.99, -4.99],
                 [-4.98, -4.98, -4.98, ..., -4.98, -4.98, -4.98],
                 [ 4.97, 4.97, 4.97, ..., 4.97, 4.97, 4.97],
[ 4.98, 4.98, 4.98, ..., 4.98, 4.98, 4.98],
[ 4.99, 4.99, 4.99, ..., 4.99, 4.99, 4.99]])
          array([[7.07106781, 7.06400028, 7.05693985, ..., 7.04988652, 7.05693985,
                  7.06400028],
                 [7.06400028, 7.05692568, 7.04985815, ..., 7.04279774, 7.04985815,
                  7.05692568],
                 [7.05693985, 7.04985815, 7.04278354, ..., 7.03571603, 7.04278354,
                  7.04985815],
                 [7.04988652, 7.04279774, 7.03571603, ..., 7.0286414, 7.03571603,
                  7.04279774],
                 [7.05693985, 7.04985815, 7.04278354, ..., 7.03571603, 7.04278354,
                  7.04985815],
                 [7.06400028, 7.05692568, 7.04985815, ..., 7.04279774, 7.04985815,
                  7.05692568]])
```

close all open plot windows by executing plt.close("all")



Expressing Conditional Logic as Array Operations

np.where: condition, x: an array or an scalar (if condition), y: an array or scalar (else condition).

```
In [28]: | xarr = np.array([1.1, 1.2, 1.3, 1.4, 1.5])
           yarr = np.array([2.1, 2.2, 2.3, 2.4, 2.5])
           cond = np.array([True, False, True, True, False])
           result = [(x if c else y) for x,y,c in zip(xarr, yarr, cond)]
           display(result)
           print('will not be very fast for large arrays; not work with multidimensional arrays')
           result = np.where(cond, xarr, yarr)
           display(result)
           arr = rng.standard_normal((4, 4))
           display(arr, arr>0)
           display(np.where(arr>0, 2, -2))
           display(np.where(arr>0, 2, arr))
           [1.1, 2.2, 1.3, 1.4, 2.5]
           will not be very fast for large arrays; not work with multidimensional arrays
           array([1.1, 2.2, 1.3, 1.4, 2.5])
           array([[ 2.61815943, 0.77736134, 0.8286332 , -0.95898831], [-1.20938829, -1.41229201, 0.54154683, 0.7519394 ], [-0.65876032, -1.22867499, 0.25755777, 0.31290292], [-0.13081169, 1.26998312, -0.09296246, -0.06615089]])
           array([[ True, True, True, False],
                    [False, False, True, True],
                    [False, False, True, True],
                    [False, True, False, False]])
           array([[ 2, 2, 2, -2],
                   [-2, -2, 2, 2],
                    [-2, -2, 2, 2],
                   [-2, 2, -2, -2]]
                   [-1.20938829, -1.41229201, 2. , -0.95898831],
[-0.65876032, -1.22867499, 2. , 2. ],
[-0.13081169, 2
           array([[ 2.
                                           , -0.09296246, -0.06615089]
```

Mathematical and Statistical Methods

In []:	
In []:	
In [29]:	# resume: page - 111
In []:	