Section 6 Introduction to Numpy

NumPy -- *Numerical Python* provides the building-blocks for the entire ecosystem of data science tools in Python, serving as the efficient tool to store and manipulate data, and friendly to Matlab users.

Unfortunately, the native numpy does not support GPU operations. For arrays on GPU, we have some popular substitutions, such as tensors in TensorFlow and jax (by Google), PyTorch (by Facebook) or arrays in CuPy (by Nvidia) -- while they all have close relations/ similar interface with Numpy. Therefore, learning the basic concepts about Numpy is crucial for doing data science with Python.

Difference between ndarray and list: Data Memory Perspective

Intuitively speaking, the built-in list object in Python can be viewed as the "address book" that store multiple pointers to heterogeneous objects in Python as its elements. On the other, the Numpy array object in Python stored the pointer to a consecutive memory block (data buffer) implemented in C language -- that's why the elements in Numpy array should be fixed-type, and the implementation is more efficient than list.

```
a = np.array([1,2,3,4]) #numpy 1-d array, initialization with list
l = [1,2,3,4] # python built-in list
```

Slicing of Numpy array creates *View* instead of *Copy*. The view object shares the same data buffer with the original one.

```
In [13]: b = a[0:2] # creating view by slicing
```

```
print(b)
In [14]:
           b.base # view has the base object because its memory is from some other object.
          [1 2]
Out[14]: array([1, 2, 3, 4])
         We can also check the flags to see whether the array has its "own data".
In [15]:
           b.flags
            C_CONTIGUOUS : True
Out[15]:
            F CONTIGUOUS : True
            OWNDATA : False
            WRITEABLE : True
            ALIGNED : True
            WRITEBACKIFCOPY : False
            UPDATEIFCOPY : False
In [16]:
           a.flags
Out[16]:
            C_CONTIGUOUS : True
            F CONTIGUOUS : True
            OWNDATA : True
            WRITEABLE: True
            ALIGNED : True
            WRITEBACKIFCOPY : False
            UPDATEIFCOPY : False
         This mechanism may cause unexpected outcomes for beginners.
In [17]:
           b[0] = 1000 \text{ # change the first element of } b \text{ (which is the slice of } a -- view)
Out[17]: array([1000,
                           2,
                                  3,
                                        4])
         This is very different with the Python built-in list.
In [18]:
           c = 1[0: 2] #slicing in list, c is a copy of l
           c[0] = 100
Out[18]: [1, 2, 3, 4]
         Many other methods/functions in Numpy creates view instead of copy (in fact view is far more
         efficient than copy).
         For example, Reshape creates the view whenever possible (for most of the case with consistent
         dimensions).
In [19]:
           a_mat = a.reshape(2,2)
           print(a_mat)
          [[1000
                     2]
                     4]]
```

```
print(a_mat[1,0]) #vertical index (top to bottom)
In [20]:
          print(a mat[0,1]) #horizontal index (left to right)
          3
          2
In [21]:
          a mat.base
Out[21]: array([1000,
                                 3,
                                       4])
                          2,
In [22]:
          a_mat[0,0] = 2000 # same as a_mat[0][0]
Out[22]: array([2000,
                          2,
                                 3,
                                       4])
         Transpose also creates the view.
In [23]:
          a_t = a_mat.T # attribute
          a_tt = a_mat.transpose() # method
          print(a t) #swapped row and column
          print(a_tt)
          [[2000
                    3]
                    4]]
               2
          [[2000
                    3]
                    4]]
               2
In [18]:
           a_t.base
Out[18]: array([2000,
                          2,
                                 3,
                                       4])
In [24]:
          a_t[0,0] = 0 # change the view -- change the data buffer -- the base a is also changed!
Out[24]: array([0, 2, 3, 4])
         Conversely, once the "base" is changed, all the associated "view" objects are changed!
In [25]:
          a mat # reshape of a -- view, changed!
Out[25]: array([[0, 2],
                 [3, 4]])
In [26]:
          b # slicing of a -- view, changed!
Out[26]: array([0, 2])
         Use the copy method to create the new data buffer
In [28]:
           a_copy = a.copy()
          print(a_copy)
           print(a_copy.base)
```

```
[0 2 3 4]
         None
In [29]:
          a copy.flags
           C_CONTIGUOUS : True
Out[29]:
           F_CONTIGUOUS : True
           OWNDATA : True
           WRITEABLE : True
           ALIGNED : True
           WRITEBACKIFCOPY : False
           UPDATEIFCOPY : False
In [30]:
          a_mat_copy = a_mat.copy()
In [31]:
          a_mat_copy.flags
           C CONTIGUOUS : True
Out[31]:
           F CONTIGUOUS : False
           OWNDATA : True
           WRITEABLE: True
           ALIGNED : True
           WRITEBACKIFCOPY : False
           UPDATEIFCOPY : False
```

Numpy ndarray as object

As the object created by Numpy, the ndarray has identity, type, value, attributes and methods.

```
In [32]:
          type(a)
         numpy.ndarray
Out[32]:
 In [ ]:
          dir(a)
 In [ ]:
          help(a)
In [35]:
          a = np.arange(4)
          print(a.shape) # 1-d array with length 4 -- different with 4x1 2-d array!
          print(a)
          (4,)
          [0 1 2 3]
In [42]:
          b = a.reshape(-1,1) #similar to how -1 is used as an index for the end of a list.
          print(b.shape)
          print(b)
          (4, 1)
          [[0]]
           [1]
```

```
[2]
           [3]]
In [43]:
          a_mat.shape
Out[43]: (2, 2)
In [47]:
          L = a_mat.tolist() #each row of matrix is an element of the new list
          print(L)
          print(L[1])
          print(L[1][0])
          [[0, 2], [3, 4]]
          [3, 4]
In [48]:
          a.mean()
Out[48]: 1.5
In [49]:
          help(a.mean)
         Help on built-in function mean:
         mean(...) method of numpy.ndarray instance
              a.mean(axis=None, dtype=None, out=None, keepdims=False, *, where=True)
              Returns the average of the array elements along given axis.
              Refer to `numpy.mean` for full documentation.
              See Also
              numpy.mean : equivalent function
In [51]:
          np.mean(a)
Out[51]: 1.5
In [39]:
          help(a.reshape)
         Help on built-in function reshape:
         reshape(...) method of numpy.ndarray instance
              a.reshape(shape, order='C')
              Returns an array containing the same data with a new shape.
              Refer to `numpy.reshape` for full documentation.
              See Also
              numpy.reshape : equivalent function
              Notes
```

Unlike the free function `numpy.reshape`, this method on `ndarray` allows the elements of the shape parameter to be passed in as separate arguments. For example, ``a.reshape(10, 11)`` is equivalent to ``a.reshape((10, 11))``.

Dimension and Axis of ndarray

Numpy uses the terms *dimension* and *axis* (indexing from 0) to describe the degree of freedom of an array. See the illustrations here.

```
In [6]:
         a = np.arange(24).reshape(2,3,4) # 3-d array, or tensor
         а
Out[6]: 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]]])
       In the method reshape, you can also pass value -1 to let Numpy calculate the number for you.
In [4]:
         np.arange(24).reshape(2,-1,4)
Out[4]: 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]]])
In [4]:
         print(a[1,0,0]) #first index is depth (from front to back)
         print(a[0,1,0]) #second index is vertical (from top to bottom), which row do you want?
         print(a[0,0,1]) #third index is horizontal (from left to right), which column do you wo
        12
        4
        1
In [5]:
         help(np.arange) # note the difference with range()
        Help on built-in function arange in module numpy:
        arange(...)
            arange([start,] stop[, step,], dtype=None, *, like=None)
            Return evenly spaced values within a given interval.
            Values are generated 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.
            When using a non-integer step, such as 0.1, the results will often not
```

```
be consistent. It is better to use `numpy.linspace` for these cases.
Parameters
start : integer or real, optional
   Start of interval. The interval includes this value. The default
   start value is 0.
stop: integer or real
    End of interval. The interval does not include this value, except
    in some cases where `step` is not an integer and floating point
    round-off affects the length of `out`.
step : integer or real, optional
   Spacing between values. For any output `out`, this is the distance
   between two adjacent values, ``out[i+1] - out[i]``. The default
    step size is 1. If `step` is specified as a position argument,
    `start` must also be given.
dtype : dtype
    The type of the output array. If `dtype` is not given, infer the data
    type from the other input arguments.
like : array like
    Reference object to allow the creation of arrays which are not
   NumPy arrays. If an array-like passed in as ``like`` supports
          __array_function__`` protocol, the result will be defined
   by it. In this case, it ensures the creation of an array object
   compatible with that passed in via this argument.
    .. note::
       The ``like`` keyword is an experimental feature pending on
        acceptance of :ref:`NEP 35 <NEP35>`.
    .. versionadded:: 1.20.0
Returns
-----
arange : ndarray
   Array of evenly spaced values.
    For floating point arguments, the length of the result is
     `ceil((stop - start)/step)``. Because of floating point overflow,
    this rule may result in the last element of `out` being greater
   than `stop`.
See Also
numpy.linspace : Evenly spaced numbers with careful handling of endpoints.
numpy.ogrid: Arrays of evenly spaced numbers in N-dimensions.
numpy.mgrid: Grid-shaped arrays of evenly spaced numbers in N-dimensions.
Examples
_____
>>> np.arange(3)
array([0, 1, 2])
```

```
array([ 0., 1., 2.])
>>> np.arange(3,7)
array([3, 4, 5, 6])
>>> np.arange(3,7,2)
array([3, 5])
```

>>> np.arange(3.0)

In [7]: print(a.T) #Exercise: Describe what happens here
a.T.shape

```
[ 4 16]
            [ 8 20]]
           [[ 1 13]
           [ 5 17]
           [ 9 21]]
           [[ 2 14]
            [ 6 18]
           [10 22]]
           [[ 3 15]
           [ 7 19]
           [11 23]]]
 Out[7]: (4, 3, 2)
 In [8]:
          a_1d = np.array([1,2,3,4])
          a_1d.shape #1 axis
 Out[8]: (4,)
 In [9]:
          a 1d.T.shape # transpose is still 1-D array! this is very different with Matlab!
 Out[9]: (4,)
In [10]:
          print(a_1d)
          print(a_1d.T)
          [1 2 3 4]
          [1 2 3 4]
In [11]:
          a_2d = a_1d[:,np.newaxis] # increase dimension. The new dimension will be the second co
          a_2d.shape
Out[11]: (4, 1)
In [11]:
          help(np.newaxis) #has no value, not a function either. This attribute just allows us to
         Help on NoneType object:
         class NoneType(object)
             Methods defined here:
              __bool__(self, /)
                  self != 0
              __repr__(self, /)
                  Return repr(self).
              Static methods defined here:
              __new__(*args, **kwargs) from builtins.type
                  Create and return a new object. See help(type) for accurate signature.
```

```
print(a_2d) #recall the first index is vertical!
In [15]:
          print(a 2d.T)
          [[1]
           [2]
           [3]
           [4]]
          [[1 2 3 4]]
In [13]:
          a 1d
Out[13]: array([1, 2, 3, 4])
In [14]:
          print(a_1d.ndim)
          print(a_2d.ndim)
         1
          2
In [18]:
          a_2d_alt = a_1d[np.newaxis,1:3]
          print(a_2d_alt)
          print(a 2d alt.shape)
          a_3d = a_1d[:,np.newaxis,np.newaxis] #tensor where orignal list is along the depth axis
          print(a_3d)
          print(a_3d.shape)
          #experiement with a 1d[np.newaxis,:,np.newaxis] a 1d[np.newaxis,np.newaxis,:], see what
          [[2 3]]
          (1, 2)
          [[[1]]
           [[2]]
           [[3]]
          [[4]]]
          (4, 1, 1)
         To change the multi-dimension array to 1-d array, in addition to reshape (create view), we can also
         choose ravel (create view) or flatten (create copy).
In [17]:
          a_mat = np.zeros((2,2)) # note the parentheses here
          a_mat_reshape = a_mat.reshape(-1) # -1 means default length -- create view
          a_mat_ravel = a_mat.ravel()
          a_mat_flatten = a_mat.flatten()
In [18]:
          a mat reshape
Out[18]: array([0., 0., 0., 0.])
In [70]:
          a mat ravel #view of a mat
Out[70]: array([0., 0., 0., 0.])
```

```
In [71]: | a_mat_flatten #copy of a_mat
Out[71]: array([0., 0., 0., 0.])
In [52]:
          a mat ravel.base
Out[52]: array([[0., 0.],
                 [0., 0.]])
In [53]:
          a mat flatten.flags
           C_CONTIGUOUS : True
Out[53]:
           F CONTIGUOUS : True
           OWNDATA : True
           WRITEABLE : True
           ALIGNED : True
           WRITEBACKIFCOPY : False
           UPDATEIFCOPY : False
```

Indexing of ndarray

1. Slicing: Similiar to the list indexing

Always remember that slicing creates the view instead of copy!

```
In [24]:
          a = np.array([[1,2,3,4], [5,6,7,8], [9,10,11,12]])
          print(a)
          b = a[:2, 1:3] # creates a view instead of copy
          print(b)
          print(a[0, 1])
          b[0, 0] = 77
          print(a[0, 1])
          print(a)
          [[1 2 3 4]
          [5 6 7 8]
          [ 9 10 11 12]]
         [[2 3]
          [6 7]]
         77
         [[ 1 77 3 4]
          [5 6 7 8]
          [ 9 10 11 12]]
         Be cautious with the difference between simple indexing (one integer index) and slicing.
```

```
[9]])
In [22]:
          a[0:1,:] # 2-d array
Out[22]: array([[ 1, 77, 3, 4]])
In [23]:
          a[0,:] #1-d array
Out[23]: array([ 1, 77, 3, 4])
         For more exercise: See Figure 4-2 in this material.
         2. Boolean Indexing
In [23]:
          a[a<5] = 0 # In Numpy terms, a<5 creates the "mask" contaning true or false values
In [24]:
Out[24]: array([[ 0, 77, 0, 0],
                 [ 5, 6, 7, 8],
[ 9, 10, 11, 12]])
In [25]:
          b = a[a>2]
Out[25]: array([77, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12])
In [26]:
          b[0] = -3
          print(b)
          print(a)
          b.flags
          [-3 3 4 5 6 7 8 9 10 11 12]
          [[ 1 77 3 4]
           [5 6 7 8]
          [ 9 10 11 12]]
           C CONTIGUOUS : True
Out[26]:
           F CONTIGUOUS : True
           OWNDATA : True
           WRITEABLE : True
           ALIGNED : True
           WRITEBACKIFCOPY : False
           UPDATEIFCOPY : False
         Boolean indexing can create new numpy ndarray instead of the view.
In [28]:
          x = np.arange(10)
          y = x[(x>4) & (x<8)] # just for your information: do not use keyword "and" here
In [29]:
Out[29]: array([5, 6, 7])
```

```
In [62]:
          y.flags
           C_CONTIGUOUS : True
Out[62]:
            F CONTIGUOUS : True
           OWNDATA : True
           WRITEABLE : True
           ALIGNED : True
           WRITEBACKIFCOPY : False
           UPDATEIFCOPY : False
         3. Integer Array Indexing (Fancy Indexing)
         General rule: arr[[ind1,ind2]] just means np.array([arr[ind1],arr[ind2]])
In [33]:
          ind = np.array([1,0,2]) # no problem for list [1,0,2]
          x = np.arange(0,10,2)
          print(x)
          x[ind] # equivalently, x[[1,0,2]]
         [0 2 4 6 8]
Out[33]: array([2, 0, 4])
In [35]:
          z = np.linspace(1,2,6) #6 evenly spaced points between 1 and 2
          print(z)
          z[ind]
         [1. 1.2 1.4 1.6 1.8 2. ]
Out[35]: array([1.2, 1. , 1.4])
In [36]:
          a = np.arange(12).reshape(3,4)
Out[36]: array([[ 0, 1, 2, 3],
                [ 4, 5, 6, 7],
[ 8, 9, 10, 11]])
In [37]:
          a[[1,0,2],:] #Rearranges the rows, keeps everything in each row
Out[37]: array([[ 4, 5, 6, 7],
                 [0, 1, 2, 3],
                [8, 9, 10, 11]])
In [38]:
          a[2,[1,0,2]] #Last row, then pull from indices on that row
Out[38]: array([ 9, 8, 10])
```

Numpy Universal Functions (ufuncs) and Aggregate Function

Similar to Matlab, the built-in loops in Python can be very slow for large-scale problems. To solve this issue, Numpy adopts vectorized methods (uses vectorization) written in optimized C-language

codes, and provides the interface as Numpy universal functions (ufuncs).

Numpy ufuncs operates on ndarrays in an element-by-element fashion. You can find all the ufuncs in the documentation.

```
In [39]:
          x = np.arange(1000000)
          np.log(1+x) #ln(1+0), ln(1+1) up to ln(1+999999)
Out[39]: array([ 0.
                            , 0.69314718, 1.09861229, ..., 13.81550856,
                 13.81550956, 13.81551056])
         We can also iterate the numpy array through elements just as Python built-in list (of course you can
         always get elements through iterating the index), although it is not very recommended for large-
         scale problems.
In [40]:
          a = np.arange(6)
          for elem in a:
              print(elem, end =" " )
         0 1 2 3 4 5
In [40]:
          help(print)
         Help on built-in function print in module builtins:
          print(...)
              print(value, ..., sep=' ', end='\n', file=sys.stdout, flush=False)
              Prints the values to a stream, or to sys.stdout by default.
              Optional keyword arguments:
              file: a file-like object (stream); defaults to the current sys.stdout.
              sep: string inserted between values, default a space.
                     string appended after the last value, default a newline.
              flush: whether to forcibly flush the stream.
In [42]:
          a = a.reshape(2,-1)
          for row in a:
              print(row, end =" " ) #default value is end ='\n', for a new line
          [0 1 2] [3 4 5]
In [18]:
          for row in a:
              for elem in row:
                   print(elem, end =" " )
         0 1 2 3 4 5
In [19]:
          for elem in np.nditer(a):
              print(elem, end =" " )
          0 1 2 3 4 5
In [20]:
          for (idx, elem) in np.ndenumerate(a):
              print([idx, elem])
```

```
[(0, 0), 0]
          [(0, 1), 1]
          [(0, 2), 2]
[(1, 0), 3]
[(1, 1), 4]
          [(1, 2), 5]
         Numpy also provides some useful aggregate functions.
In [41]:
           a = np.arange(6).reshape(2,3)
Out[41]: array([[0, 1, 2],
                 [3, 4, 5]])
In [42]:
           a.sum(axis=0)
Out[42]: array([3, 5, 7])
In [43]:
           a.sum(axis=1)
Out[43]: array([ 3, 12])
In [44]:
           a.sum()
Out[44]: 15
In [45]:
           a.min(axis=1)
Out[45]: array([0, 3])
In [46]:
           b = np.arange(24).reshape(2,3,-1)
           b
Out[46]: 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]]])
In [47]:
           b.sum(axis=1) #column sum, 8 columns in this tensor
Out[47]: array([[12, 15, 18, 21],
                  [48, 51, 54, 57]])
In [48]:
           b.max(axis=0) #max along depth axis.
Out[48]: array([[12, 13, 14, 15],
                 [16, 17, 18, 19],
[20, 21, 22, 23]])
```

Numpy Linear Algebra Functions

See the reference here and compare it with Matlab. Be cautious with operators like *, @ (only available after Python 3.5) and functions/methods dot, vdot and matmul.

```
In [72]:
          help(np.dot)
         Help on function dot in module numpy:
         dot(...)
             dot(a, b, out=None)
             Dot product of two arrays. Specifically,
             - If both `a` and `b` are 1-D arrays, it is inner product of vectors
               (without complex conjugation).
              - If both `a` and `b` are 2-D arrays, it is matrix multiplication,
               but using :func:`matmul` or ``a @ b`` is preferred.
              - If either `a` or `b` is 0-D (scalar), it is equivalent to :func:`multiply`
               and using ``numpy.multiply(a, b)`` or ``a * b`` is preferred.
              - If `a` is an N-D array and `b` is a 1-D array, it is a sum product over
               the last axis of `a` and `b`.
             - If `a` is an N-D array and `b` is an M-D array (where ``M>=2``), it is a
               sum product over the last axis of `a` and the second-to-last axis of `b`::
                 dot(a, b)[i,j,k,m] = sum(a[i,j,:] * b[k,:,m])
             Parameters
              -----
             a : array like
                 First argument.
             b : array_like
                 Second argument.
             out : ndarray, optional
                 Output argument. This must have the exact kind that would be returned
                 if it was not used. In particular, it must have the right type, must be
                 C-contiguous, and its dtype must be the dtype that would be returned
                 for `dot(a,b)`. This is a performance feature. Therefore, if these
                 conditions are not met, an exception is raised, instead of attempting
                 to be flexible.
             Returns
             output : ndarray
                 Returns the dot product of `a` and `b`. If `a` and `b` are both
                 scalars or both 1-D arrays then a scalar is returned; otherwise
                 an array is returned.
                 If `out` is given, then it is returned.
             Raises
             ValueError
                 If the last dimension of `a` is not the same size as
                 the second-to-last dimension of `b`.
             See Also
              _ _ _ _ _ _ _
```

vdot : Complex-conjugating dot product.

```
tensordot : Sum products over arbitrary axes.
    einsum : Einstein summation convention.
    matmul : '@' operator as method with out parameter.
    Examples
    >>> np.dot(3, 4)
    Neither argument is complex-conjugated:
    >>> np.dot([2j, 3j], [2j, 3j])
    (-13+0j)
    For 2-D arrays it is the matrix product:
    >>> a = [[1, 0], [0, 1]]
    \Rightarrow b = [[4, 1], [2, 2]]
    >>> np.dot(a, b)
    array([[4, 1],
           [2, 2]])
    \Rightarrow a = np.arange(3*4*5*6).reshape((3,4,5,6))
    >>> b = np.arange(3*4*5*6)[::-1].reshape((5,4,6,3))
    >>> np.dot(a, b)[2,3,2,1,2,2]
    499128
    >>> sum(a[2,3,2,:] * b[1,2,:,2])
    499128
help(np.vdot)
Help on function vdot in module numpy:
vdot(...)
    vdot(a, b)
    Return the dot product of two vectors.
    The vdot(`a`, `b`) function handles complex numbers differently than
    dot(`a`, `b`). If the first argument is complex the complex conjugate
    of the first argument is used for the calculation of the dot product.
    Note that `vdot` handles multidimensional arrays differently than `dot`:
    it does *not* perform a matrix product, but flattens input arguments
    to 1-D vectors first. Consequently, it should only be used for vectors.
    Parameters
    a : array like
        If `a` is complex the complex conjugate is taken before calculation
        of the dot product.
    b : array like
        Second argument to the dot product.
    Returns
    _ _ _ _ _ _
    output : ndarray
        Dot product of `a` and `b`. Can be an int, float, or
        complex depending on the types of `a` and `b`.
    See Also
    dot : Return the dot product without using the complex conjugate of the
```

In [73]:

first argument.

```
Examples
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            >>> a = np.array([1+2j,3+4j])
            >>> b = np.array([5+6j,7+8j])
            >>> np.vdot(a, b)
            (70-8j)
            >>> np.vdot(b, a)
            (70+8j)
            Note that higher-dimensional arrays are flattened!
            >>> a = np.array([[1, 4], [5, 6]])
            >>> b = np.array([[4, 1], [2, 2]])
            >>> np.vdot(a, b)
            30
            >>> np.vdot(b, a)
            >>> 1*4 + 4*1 + 5*2 + 6*2
            30
In [ ]:
         help(np.matmul)
In [ ]:
```