Broadcasting

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Dimension compatibility

When operating on two arrays, NumPy compares their shapes element-wise. It starts with the trailing dimensions and works its way forward. Two dimensions are compatible when

1. they are equal; or
2. one of them is 1.

Arrays of different dimensionality

All dimensions of lower dimensionality array match **trailing** dimensions of the other. Scale the 3 color layers in an RGB image by different amounts:

Image	(3d array):	256	x	256	x	3	
Scales	(1d array):					3	$\begin{bmatrix} 1. & .9 & 1.4 \end{bmatrix}$
Result	(3d array):	256	x	256	x	3	

Trailing dimensions don't match

```
>>> import numpy as np
>>> A, B = np.arange(20).reshape((5,4)),np.arange(4)
>>> Result1 = A * B
>>> C = np.arange(5)
>>> Result2 = A * C
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: operands could not be broadcast together with shape
```

Two mismatched 1D arrays

ValueError: operands could not be broadcast together

```
>>> A1d, B1d = np.arange(4),np.arange(5)
>>> A1d + B1d
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: operands could not be broadcast together with shape
```

Examples

A	5	x	4			A	5	x	4		
B			4			B			1	Scalar!	
Result	5	x	4			Result	5	x	4		

A	15	x	3	x	5	A	15	x	3	x	5
B	15	x	1	x	5	B			3	x	5
Result	15	x	3	x	5	Result	15	x	3	x	5

Multiply by 5

$$5 \qquad + \qquad \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix}$$

$$\Downarrow$$

$$\begin{bmatrix} 5 & 5 & 5 & 5 \\ 5 & 5 & 5 & 5 \end{bmatrix} \qquad + \qquad \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix}$$

Two Matched 2D arrays

```
>>> a = np.arange(4)[:,np.newaxis]
>>> b = np.arange(5)[np.newaxis,:]
>>> print(a,a.shape)
[[0]
 [1]
 [2]
 [3]] (4, 1)
>>> print(b,b.shape)
[[0 1 2 3 4]] (1, 5)
>>> print((a+b).shape)
(4, 5)
```

"Outer" addition

a is 4x1, b is 1x5.

```
>>> print(a + b)
[[0 1 2 3 4]
 [1 2 3 4 5]
 [2 3 4 5 6]
 [3 4 5 6 7]]
```

```
r,c = a.shape[0],b.shape[1]
M = np.zeros((r,c),dtype=int)
for i in range(r):
    for j in range(c):
        M[i,j] = a[i,0] + b[0,j]
```

Broadcasting: size-one dimensions copied

4 x 1

$$\begin{bmatrix}[0]\\ [1]\\ [2]\\ [3]\end{bmatrix} \Longrightarrow \begin{bmatrix}[0 & 0 & 0 & 0 & 0]\\ [1 & 1 & 1 & 1 & 1]\\ [2 & 2 & 2 & 2 & 2]\\ [3 & 3 & 3 & 3 & 3]\end{bmatrix}$$

1 x 5

$$\begin{bmatrix}[0 & 1 & 2 & 3 & 4]\end{bmatrix}$$

$$\Downarrow$$

$$\begin{bmatrix}[0 & 1 & 2 & 3 & 4]\\ [0 & 1 & 2 & 3 & 4]\\ [0 & 1 & 2 & 3 & 4]\\ [0 & 1 & 2 & 3 & 4]\end{bmatrix}$$

Shapes?

```
>>> import numpy as np
>>> a1d, b1d = np.arange(4),np.arange(5)
>>> a, b = a1d.reshape((4,1)), b1d.reshape((5,1))
```

```
>>> a1d_p_b = a1d + b
>>> a_p_b1d = a + b1d
```

Values

```
>>> print(a.shape, b.shape)
(4, 1) (5, 1)
>>> a1d_p_b
array([[0, 1, 2, 3],
       [1, 2, 3, 4],
       [2, 3, 4, 5],
       [3, 4, 5, 6],
       [4, 5, 6, 7]])
>>> a_p_b1d
array([[0, 1, 2, 3, 4],
       [1, 2, 3, 4, 5],
       [2, 3, 4, 5, 6],
       [3, 4, 5, 6, 7]])
```

K Nearest Neighbors

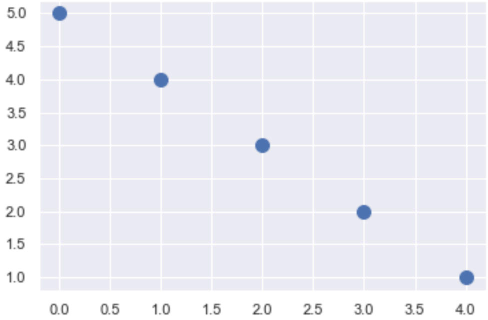
1. To illustrate the power of broadcasting with a somewhat more practical example, we'll compute the **K Nearest Neighbors** (KNN) for a set of points, where is an integer.
2. Typically the KNN problem is solved for points in a high dimensional space; each point represents a sample; each coordinate represents a value for some numerical feature of the sample. For presentational purposes we'll solve KNN for a small set of 2D points.
3. The KNN problem is important in a number of applications. For example, in a machine learning context, one strategy for classifying point X is to find the KNNs of X from among a set of points whose classes are known, and let the KNNs "vote" on the class of X.

VanderPlas's K-Nearest Neighbor calculation

```
>>> Y = (np.array([np.arange(5),np.arange(5,0,-1)])).T
>>> Y
array([[0, 5],
       [1, 4],
       [2, 3],
       [3, 2],
       [4, 1]])
>>> Y[:, np.newaxis, :].shape, Y[np.newaxis, :, :].shape
((5, 1, 2), (1, 5, 2))
>>> deltas = Y[:,np.newaxis,:] - Y[np.newaxis,:,:] # (5, 5, 2)
>>> deltas[0,:,1]  #  Y-coord diffs for Pt 0
array([0, 1, 2, 3, 4])
```

The points

$$\mathrm{dist}(\mathrm{Y}[i], \mathrm{Y}[j])^2 = (\mathrm{deltas}[i][j][0])^2 + (\mathrm{deltas}[i][j][1])^2$$



Distance calc completed (looplessly)

```
>>> dists = np.sum(deltas**2, axis=2) # x**2 lyr + y**2 lyr
>>> print(dists) # dists[i,j] = sqd dist from i to j
[[ 0  2  8 18 32]
 [ 2  0  2  8 18]
 [ 8  2  0  2  8]
 [18  8  2  0  2]
 [32 18  8  2  0]]
>>> nearest = np.argsort(dists, axis=1)
>>> print(nearest) # nearest[i,:] = sorted nbrs of point i
[[0 1 2 3 4]
 [1 0 2 3 4]
 [2 1 3 0 4]
 [3 2 4 1 0]
 [4 3 2 1 0]]
```

Finding the K nearest ($k = 2$)

Less work: Partition the set of points into the top $K + 1$ ($k = 2$) and all the rest:

```
>>> nearest_k = np.argpartition(dists, kth = 3, axis=1)
>>> print(nearest_k) # nearest[i,:k] = unsorted K nearest nbrs
[[1 0 2 3 4]
 [1 2 0 3 4]
 [3 2 1 0 4]
 [3 2 4 1 0]
 [3 4 2 1 0]]
```

Takeaways

1. Basic ‘numpy‘ op: elementwise arithmetic between ‘ndarray‘s of the same shape.
2. Broadcasting licenses stretching operations on dimensions of size 1, or lower dimensionality arrays when “trailing” dimensions match.
3. The broadcasting operation can be used to achieve the effect of a loop, performing a single operation on all the elements. To achieve this we sometimes increase the dimensionality of the data (‘:newaxis‘].
4. Complementing broadcasting (in the KNN example):
    - U-functions (universal functions) [‘deltas**2‘]
    - Aggregation operations [‘np.sum(deltas**2, axis=2)‘]