Scientific Computing with Python

Feng Chen
HPC User Services
LSU HPC & LONI
sys-help@loni.org

Louisiana State University
Baton Rouge
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Outline

- **Day 1 Basic Python Review**
- **Introducing Python Modules:**
  - Numpy
  - Scipy
- **Examples**
  - Calculate derivative of a function
  - Convert RGB image to Grayscale
  - Simple regression example
- **Exercise and Mini-Project**
  - Numpy warmup exercise
  - Calculate k nearest neighbor of image data

Day 1 Basic Python Recap

- **Python is a general-purpose interpreted, interactive, object-oriented, and high-level programming language.**
- **It was created by Guido van Rossum during 1985-1990. Like Perl, Python source code is also available under the GNU General Public License (GPL).**

Advantage of using Python

- **Python is:**
  - Interpreted:
    - Python is processed at runtime by the interpreter. You do not need to compile your program before executing it. This is similar to PERL and PHP.
  - Interactive:
    - You can actually sit at a Python prompt and interact with the interpreter directly to write your programs.
  - Object-Oriented:
    - Python supports Object-Oriented style or technique of programming that encapsulates code within objects.
  - Beginner's Language:
    - Python is a great language for the beginner-level programmers and supports the development of a wide range of applications from simple text processing to browsers to games.

Directly Run into List/Array

```
#!/usr/bin/env python
# generate array from 0-4
a = list(range(5))
print(a)
# len(a)=5
for idx in range(len(a)):
    a[idx] += 5
print(a)
```

```
[fchen14@shelob001 python]$ ./loop_array.py
[0, 1, 2, 3, 4]
[5, 6, 7, 8, 9]
```

Python Tuples

- **A Python tuple is a sequence of immutable Python objects. Creating a tuple is as simple as putting different comma-separated values.**

```
#!/usr/bin/env python
tup1 = ('physics', 'chemistry', 1997, 2000);
tup2 = (1, 2, 3, 4, 5 );
tup3 = "a", "b", "c", "d";
# The empty tuple is written as two parentheses containing nothing
tup1 = ();
# To write a tuple containing a single value you have to include a comma,
tup1 = (50,);
# Accessing Values in Tuples
print("tup1[0]: ", tup1[0])
print("tup2[1:5]: ", tup2[1:5])
# Updating Tuples, create a new tuple as follows
tup3 = tup1 + tup2;
print(tup3)
# delete tuple elements
del tup3;
print("After deleting tup3 : ")
print(tup3)
```

Scientific Computing using Python

Introducing Numpy

Numpy Overview

- **NumPy (Numeric Python) is the core package for scientific computing in Python.**
- **It is a Python library that provides a multidimensional array object, various derived objects (such as masked arrays and matrices)**
- **An assortment of routines for fast operations on arrays, including mathematical, logical, shape manipulation, sorting, selecting, I/O, discrete Fourier transforms, basic linear algebra, basic statistical operations, random simulation and much more.**

- **NumPy package provides basic routines for manipulating large arrays and matrices of numeric data.**

Basic Array Operations

- **Simple array math using np.array**
- **Note that NumPy array starts its index from *0*, end at *N-1* (C-style)**

```
# To avoid module name collision inside package context
>>> import numpy as np
>>> a = np.array([1,2,3])
>>> b = np.array([4,5,6])
>>> a+b
array([5, 7, 9])
>>> a*b
array([ 4, 10, 18])
>>> a ** b
array([  1,  32, 729])
```

Setting Array Element Values

```
>>> a[0]
1
>>> a[0]=11
>>> a
array([11,  2,  3,  4])
>>> a.fill(0) # set all values in the array with 0
>>> a[:]=1 # why we need to use [:]?
>>> a
array([1, 1, 1, 1])
>>> a.dtype   # note that a is still int64 type !
dtype('int64')
>>> a[0]=10.6 # decimal parts are truncated, be careful!
>>> a
array([10,  1,  1,  1])
>>> a.fill(-3.7) # fill() will have the same behavior
>>> a
array([-3, -3, -3, -3])
```

Numpy Array Properties (1)

```
>>> a = np.array([0,1,2,3]) # create a from a list
# create evenly spaced values within [start, stop)
>>> a = np.arange(1,5)
>>> a
array([1, 2, 3, 4])
>>> type(a)
<type 'numpy.ndarray'>
>>> a.dtype
dtype('int64')
# Length of one array element in bytes
>>> a.itemsize
8
```

Numpy Array Properties (2)

```
# shape returns a tuple listing the length of the array
# along each dimension.
>>> a.shape # or np.shape(a)
>>> a.size  # or np.size(a), return the total number of elements
4
# return the number of bytes used by the data portion of the array
>>> a.nbytes
32
# return the number of dimensions of the array
>>> a.ndim
1
```

Numpy Array Creation Functions (1)

```
# Nearly identical to Python’s
range(). Creates an array of values
in the range [start,stop) with the
specified step value. Allows non-
integer values for start, stop, and
step. Default dtype is derived from
the start, stop, and step values.
>>> np.arange(4)
array([0, 1, 2, 3])
>>> np.arange(0, 2*np.pi, np.pi/4)
array([ 0.,  0.78539816,  1.57079633,
2.35619449,  3.14159265,  3.92699082,
4.71238898,  5.49778714])
>>> np.arange(1.5,2.1,0.3)
array([ 1.5,  1.8,  2.1])
# ONES, ZEROS
# ones(shape, dtype=float64)
# zeros(shape, dtype=float64)
# shape is a number or sequence
```

```
# specifying the dimensions of the
# array. If dtype is not specified,
# it defaults to float64.
>>> a=np.ones((2,3))
>>> a
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
>>> a.dtype
dtype('float64')
>>> a=np.zeros(3)
>>> a
array([ 0.,  0.,  0.])
>>> a.dtype
dtype('float64')
```

Numpy Array Creation Functions (2)

```
# Generate an n by n identity
# array. The default dtype is
# float64.
>>> a = np.identity(4)
>>> a
array([[ 1.,  0.,  0.,  0.],
       [ 0.,  1.,  0.,  0.],
       [ 0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  1.]])
>>> a.dtype
dtype('float64')
>>> np.identity(4, dtype=int)
array([[1, 0, 0, 0],
       [0, 1, 0, 0],
       [0, 0, 1, 0],
       [0, 0, 0, 1]])
# empty(shape, dtype=float64,
# order='C')
```

```
>>> a = np.empty(2)
>>> a
array([ 0.,  0.])
# fill array with 5.0
>>> a.fill(5.0)
>>> a
array([ 5.,  5.])
# alternative approach
# (slightly slower)
>>> a[:] = 4.0
>>> a
array([ 4.,  4.])
```

Numpy Array Creation Functions (3)

```
# Generate N evenly spaced elements between (and including)
# start and stop values.
>>> np.linspace(0,1,5)
array([ 0.  ,  0.25,  0.5 ,  0.75,  1.  ])
# Generate N evenly spaced elements on a log scale between
# base**start and base**stop (default base=10).
>>> np.logspace(0,1,5)
array([  1., 1.77827941, 3.16227766,   5.62341325, 10.])
```

Array from/to ASCII files

- **Useful tool for generating array from txt file**
  - `loadtxt`
  - `genfromtxt`
- **Consider the following example:**

```
#  data.txt
Index
Brain Weight
Body Weight
#here is the training set
 1     3.385    44.500 abjhk
 2     0.480    33.38  bc_00asdk
 ...
#here is the cross validation set
 6    27.660   115.000 rk
 7    14.830    98.200 fff
 ...
 9     4.190    58.000 kij
```

Using loadtxt and genfromtxt

```
>>> a= np.loadtxt('data.txt',skiprows=16,usecols={0,1,2},dtype=None,comments="#")
>>> a
array([[   1.   ,    3.385,   44.5  ],
       [   2.   ,    0.48 ,   33.38 ],
       [   3.   ,    1.35 ,    8.1  ],
       [   4.   ,  465.   ,  423.   ],
       [   5.   ,   36.33 ,  119.5  ],
       [   6.   ,   27.66 ,  115.   ],
       [   7.   ,   14.83 ,   98.2  ],
       [   8.   ,    1.04 ,    5.5  ],
       [   9.   ,    4.19 ,   58.   ]])
# np.genfromtxt can guess the actual type of your columns by using dtype=None
>>> a= np.genfromtxt('data.txt',skip_header=16,dtype=None)
>>> a
array([(1, 3.385, 44.5, 'abjhk'), (2, 0.48, 33.38, 'bc_00asdk'),
       (3, 1.35, 8.1, 'fb'), (4, 465.0, 423.0, 'cer'),
       (5, 36.33, 119.5, 'rg'), (6, 27.66, 115.0, 'rk'),
       (7, 14.83, 98.2, 'fff'), (8, 1.04, 5.5, 'zxs'),
       (9, 4.19, 58.0, 'kij')],
      dtype=[('f0', '<i8'), ('f1', '<f8'), ('f2', '<f8'), ('f3', 'S9')])
```

Reshaping arrays

```
>>> a = np.arange(6)
>>> a
array([0, 1, 2, 3, 4, 5])
>>> a.shape
(6,)
>>> a.shape = (2,3) # reshape array to 2x3
>>> a
array([[0, 1, 2],
       [3, 4, 5]])
>>> a.reshape(3,2)  # reshape array to 3x2
array([[0, 1],
       [2, 3],
       [4, 5]])
>>> a.reshape(2,5)  # cannot change the number of elements in the array
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: total size of new array must be unchanged
>>> a.reshape(2,-1)  # numpy determines the last dimension
```

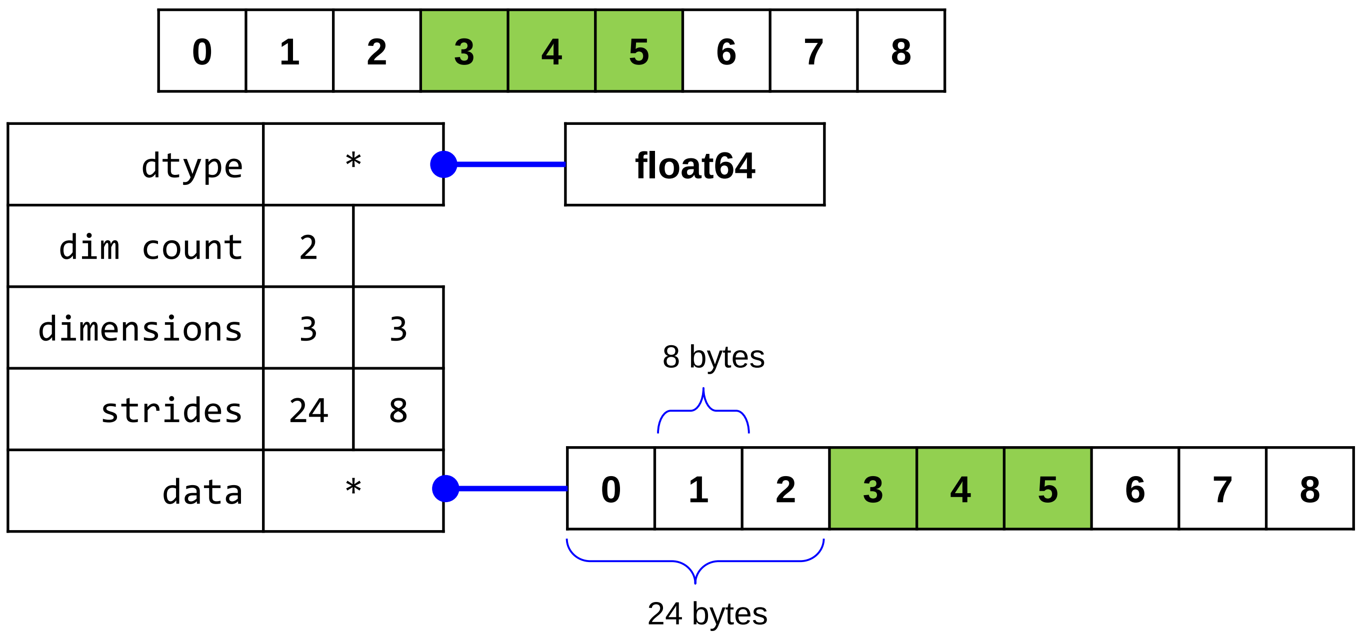
Numpy Array Data Structure

- **Numpy view of 2D array**

```
>>> a=arange(9).reshape(3,-1)
>>> a.strides
(24, 8)
>>> a.ndim
2
```

0	1	2
4	5	6
7	8	9

- **Memory block of the 2D array**



Flattening Multi-dimensional Arrays

```
# Note the difference between
# a.flatten() and a.flat
>>> a
array([[1, 2, 3],
       [4, 5, 6]])
# a.flatten() converts a
# multidimensional array into
# a 1-D array. The new array is a
# copy of the original data.
>>> b = a.flatten()
>>> b
array([1, 2, 3, 4, 5, 6])
>>> b[0] = 7
>>> b
array([7, 2, 3, 4, 5, 6])
>>> a
array([[1, 2, 3],
       [4, 5, 6]])
```

```
# a.flat is an attribute that
# returns an iterator object that
# accesses the data in the multi-
# dimensional array data as a 1-D
# array. It references the original
# memory.
>>> a.flat
<numpy.flatiter object at 0x1421c40>
>>> a.flat[:]
array([1, 2, 3, 4, 5, 6])
>>> b = a.flat
>>> b[0] = 7
>>> a
array([[7, 2, 3],
       [4, 5, 6]])
```

(Un)raveling Multi-dimensional Arrays

```
>>> a
array([[7, 2, 3],
       [4, 5, 6]])
# ravel() is the same as flatten
# but returns a reference of the
# array if possible
>>> b = a.ravel()
>>> b
array([7, 2, 3, 4, 5, 6])
>>> b[0] = 13
>>> b
array([13,  2,  3,  4,  5,  6])
>>> a
array([[13,  2,  3],
       [ 4,  5,  6]])
```

```
>>> at = a.transpose()
>>> at
array([[13,  4],
       [ 2,  5],
       [ 3,  6]])
>>> b = at.ravel()
>>> b
array([13,  4,  2,  5,  3,  6])
>>> b[0]=19
>>> b
array([19,  4,  2,  5,  3,  6])
>>> a
array([[13,  2,  3],
       [ 4,  5,  6]])
```

Four Tools in Numpy

- **Removing loops using NumPy**
  1) Ufunc (Universal Function)
  2) Aggregation
  3) Broadcasting
  4) Slicing, masking and fancy indexing

Numpy's Universal Functions

- **Numpy's universal function (or ufunc for short) is a function that operates on ndarrays in an element-by-element fashion**
- **Ufunc is a "vectorized" wrapper for a function that takes a fixed number of scalar inputs and produces a fixed number of scalar outputs.**
  - Vectorization (simplified): is the process of rewriting a loop so that instead of processing a single element of an array N times, it processes (say) 4 elements of the array simultaneously N/4 times.
- **Many of the built-in functions are implemented in compiled C code.**
  - They can be much faster than the code on the Python level

Ufunc Is Very Fast!

- **Loop version**

```
a=list(range(100000))
timeit [val+5 for val in a]
100 loops, best of 3: 4.94 ms per loop
```

- **Ufunc version**

```
a=np.array(a)
timeit a+5
10000 loops, best of 3: 98 µs per loop
```

- **Speedup**

  – 4.94 ms / 98 µs=50 !

Ufunc: Math Functions on Numpy Arrays

```
>>> x = np.arange(5.)
>>> x
array([ 0.,  1.,  2.,  3.,  4.])
>>> c = np.pi
>>> x *= c
array([  0.        ,   3.14159265,   6.28318531,   9.42477796,
12.56637061])
>>> y = np.sin(x)
>>> y
array([  0.00000000e+00,   1.22464680e-16,  -2.44929360e-16,
         3.67394040e-16,  -4.89858720e-16])
>>> import math
>>> y = math.sin(x) # must use np.sin to perform array math
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: only length-1 arrays can be converted to Python scalars
```

Ufunc: Many ufuncs available

- **Arithmetic Operators:** `+ - * / // % **`
- **Bitwise Operators:** `& | ~ ^ >> <<`
- **Comparison Oper's:** `< > <= >= == !=`
- **Trig Family:** `np.sin, np.cos, np.tan ...`
- **Exponential Family:** `np.exp, np.log, np.log10 ...`
- **Special Functions:** `scipy.special.*`
- **. . . and many, many more.**

Aggregation Functions

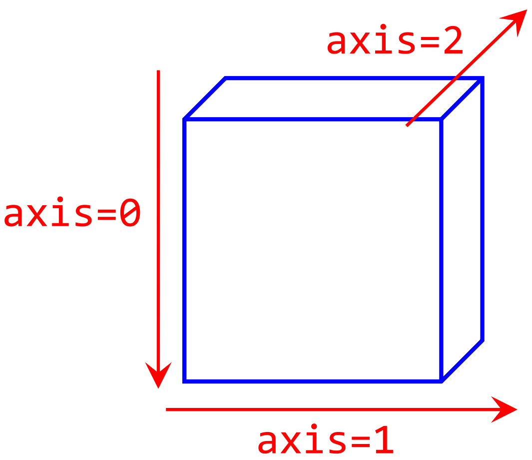
- **Aggregations are functions which summarize the values in an array (e.g. min, max, sum, mean, etc.)**
- **Numpy aggregations are much faster than Python built-in functions**

Numpy Aggregation - Array Calculation

```
>>> a=np.arange(6).reshape(2,-1)
>>> a
array([[0, 1, 2],
       [3, 4, 5]])
# by default a.sum() adds up all values
>>> a.sum()
15
# same result, functional form
>>> np.sum(a)
15
# note this is not numpy's sum!
>>> sum(a)
array([3, 5, 7])
# not numpy's sum either!
>>> sum(a,axis=0)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: sum() takes no keyword
arguments
```

```
# sum along different axis
>>> np.sum(a,axis=0)
array([3, 5, 7])
>>> np.sum(a,axis=1)
array([ 3, 12])
>>> np.sum(a,axis=-1)
array([ 3, 12])
# product along different axis
>>> np.prod(a,axis=0)
array([ 0,  4, 10])
>>> a.prod(axis=1)
array([ 0, 60])
```

The **axes** of an array describe the order of indexing into the array, e.g., axis=0 refers to the first index coordinate, axis=1 the second, etc.



Numpy Aggregation – Statistical Methods

```
>>> np.set_printoptions(precision=4)
# generate 2x3 random float array
>>> a=np.random.random(6).reshape(2,3)
>>> a
array([[ 0.7639,  0.6408,  0.9969],
       [ 0.5546,  0.5764,  0.1712]])
>>> a.mean(axis=0)
array([ 0.6592,  0.6086,  0.5841])
>>> a.mean()
0.61730865425015347
>>> np.mean(a)
0.61730865425015347
# average can use weights
>>> np.average(a,weights=[1,2,3],axis=1)
array([ 0.8394,  0.3702])
# standard deviation
>>> a.std(axis=0)
array([ 0.1046,  0.0322,  0.4129])
```

```
# variance
>>> np.var(a, axis=1)
array([ 0.0218,  0.0346])
>>> a.min()
0.17118969968007625
>>> np.max(a)
0.99691892655137737
# find index of the minimum
>>> a.argmin(axis=0)
array([1, 1, 1])
>>> np.argmax(a,axis=1)
array([2, 1])
# this will return flattened index
>>> np.argmin(a)
5
>>> a.argmax()
2
```

Numpy’s Aggregation - Summary

- **All have the same call style.**
  - `np.min() np.max() np.sum() np.prod()`
  - `np.argsort()`
  - `np.mean() np.std() np.var() np.any()`
  - `np.all() np.median() np.percentile()`
  - `np.argmin() np.argmax() . . .`
  - `np.nanmin() np.nanmax() np.nansum(). . .`

Array Broadcasting

- Broadcasting is a set of rules by which ufuncs operate on arrays of different sizes and/or dimensions.
- Broadcasting allows NumPy arrays of different dimensionality to be combined in the same expression.
- Arrays with smaller dimension are broadcasted to match the larger arrays, without copying data.

Broadcasting Rules

1. If array shapes differ, left-pad the smaller shape with 1s
2. If any dimension does not match, broadcast the dimension with size=1
3. If neither non-matching dimension is 1, raise an error.

```
np.arange(3) + 5
```

$$\begin{bmatrix}0 & 1 & 2\end{bmatrix} + \begin{bmatrix}5\end{bmatrix} = \begin{bmatrix}0 & 1 & 2\end{bmatrix} + \begin{bmatrix}5 & 5 & 5\end{bmatrix} = \begin{bmatrix}5 & 6 & 7\end{bmatrix}$$

```
np.ones((3,3)) + np.arange(3)
```

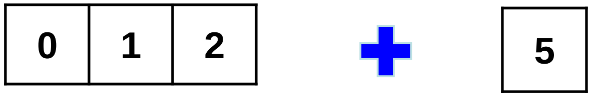
$$\begin{bmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{bmatrix} + \begin{bmatrix}0 & 1 & 2\end{bmatrix} = \begin{bmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{bmatrix} + \begin{bmatrix}0 & 1 & 2\\ 0 & 1 & 2\\ 0 & 1 & 2\end{bmatrix} = \begin{bmatrix}1 & 2 & 3\\ 1 & 2 & 3\\ 1 & 2 & 3\end{bmatrix}$$

```
np.arange(3).reshape(3,1) + np.arange(3)
```

$$\begin{bmatrix}0\\ 1\\ 2\end{bmatrix} + \begin{bmatrix}0 & 1 & 2\end{bmatrix} = \begin{bmatrix}0 & 0 & 0\\ 1 & 1 & 1\\ 2 & 2 & 2\end{bmatrix} + \begin{bmatrix}0 & 1 & 2\\ 0 & 1 & 2\\ 0 & 1 & 2\end{bmatrix} = \begin{bmatrix}0 & 1 & 2\\ 1 & 2 & 3\\ 2 & 3 & 4\end{bmatrix}$$

Broadcasting Rules – 1D array

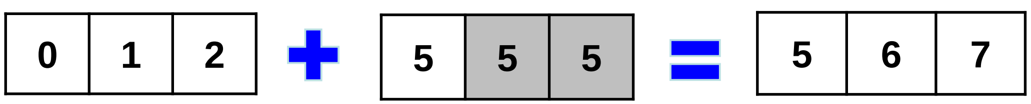
```
np.arange(3) + 5
```



1. **If array shapes differ, left-pad the smaller shape with 1s**

```
1) shape=(3,)       shape=()
2) shape=(3,)       shape=(1,)
3) shape=(3,)       shape=(3,)
4) final shape=(3,)
```

2. **If any dimension does not match, broadcast the dimension with size=1**
3. **If neither non-matching dimension is 1, raise an error.**



Broadcasting Rules – 2D array (1)

```
np.ones((3,3)) + np.arange(3)
```

1	1	1
1	1	1
1	1	1

+

0	1	2
0	1	2
0	1	2

=

1	2	3
1	2	3
1	2	3

```
1) shape=(3,3)     shape=(3,)
2) shape=(3,3)     shape=(1,3)
3) shape=(3,3)     shape=(3,3)
final shape=(3,3)
```

1. **If array shapes differ, left-pad the smaller shape with 1s**
2. **If any dimension does not match, broadcast the dimension with size=1**
3. **If neither non-matching dimension is 1, raise an error.**

Broadcasting Rules – 2D array (2)

```
np.arrange(3).reshape(3,1) + np.arange(3)
```

0	0	0
1	1	1
2	2	2

\+

0	1	2
0	1	2
0	1	2

=

0	1	2
1	2	3
2	3	4

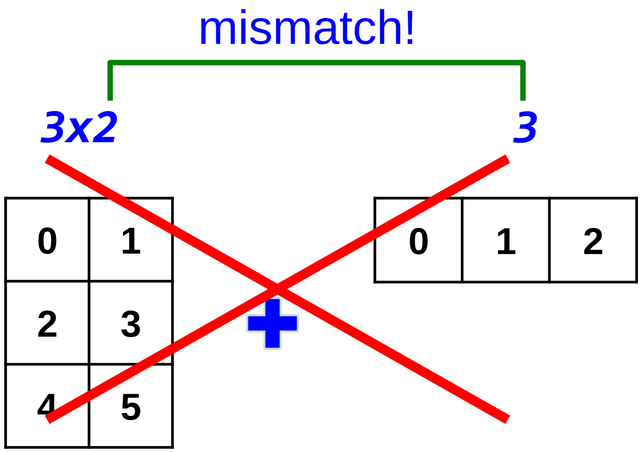
```
1) shape=(3,1)     shape=(3)
2) shape=(3,1)     shape=(1,3)
3) shape=(3,3)     shape=(3,3)
final shape=(3,3)
```

1. **If array shapes differ, left-pad the smaller shape with 1s**
2. **If any dimension does not match, broadcast the dimension with size=1**
3. **If neither non-matching dimension is 1, raise an error.**

Broadcasting Rules – Error

- **The trailing axes of either arrays must be 1 or both must have the same size for broadcasting to occur. Otherwise, a "`ValueError: operands could not be broadcast together with shapes`" exception is thrown.**

```
>>> a=np.arange(6).reshape(3,2)
>>> a
array([[0, 1],
       [2, 3],
       [4, 5]])
>>> b=np.arange(3)
>>> b
array([0, 1, 2])
>>> a+b
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: operands could not be broadcast together with shapes (3,2) (3,)
```



Slicing, Masking and Fancy Indexing

- **See next few slides...**

Array Slicing (1)

- `arr[lower:upper:step]`
- **Extracts a portion of a sequence by specifying a lower and upper bound. The lower-bound element is included, but the upper-bound element is not included. Mathematically: `[lower, upper)`. The step value specifies the stride between elements.**

```
# indices:           0  1  2  3  4
# negative indices:-5 -4 -3 -2 -1
>>> a =  np.array([10,11,12,13,14])
# The following slicing results are the same
>>> a[1:3]
array([11, 12])
>>> a[1:-2]
array([11, 12])
>>> a[-4:3]
array([11, 12])
```

Array Slicing (2)

- **Omitting Indices: omitted boundaries are assumed to be the beginning or end of the list, compare the following results**

```
>>> a[:3] # first 3 elements
array([10, 11, 12])
>>> a[-2:] # last 2 elements
array([13, 14])
>>> a[1:]  # from 1st element to the last
array([11, 12, 13, 14])
>>> a[:-1] # from 1st to the second to last
array([10, 11, 12, 13])
>>> a[:]   # entire array
array([10, 11, 12, 13, 14])
>>> a[::2] # from 1st, every other element (even indices)
array([10, 12, 14])
>>> a[1::2] # from 2nd, every other element (odd indices)
array([11, 13])
```

Multidimensional Arrays

- **A few 2D operations similar to the 1D operations shown above**

```
>>> a = np.array([[ 0, 1, 2, 3],[10,11,12,13]], float)
>>> a
array([[  0.,   1.,   2.,   3.],
       [ 10.,  11.,  12.,  13.]])
>>> a.shape # shape = (rows, columns)
(2, 4)
>>> a.size  # total elements in the array
8
>>> a.ndim  # number of dimensions
2
>>> a[1,3]  # reference a 2D array element
13
>>> a[1,3] = -1 # set value of an array element
>>> a[1]    # address second row using a single index
array([10., 11., 12., -1.])
```

2D Array Slicing

```
>>> a = np.arange(1,26)
>>> a = a.reshape(5,5) # generate the 2D array
>>> a[0,3:5]
array([4, 5])
>>> a[0,3:4]
array([4])
>>> a[4:,4:]
array([[25]])
>>> a[3:,3:]
array([[19, 20],
       [24, 25]])
>>> a[:,2]
array([ 3,  8, 13, 18, 23])
>>> a[2::2,::2]
array([[11, 13, 15],
       [21, 23, 25]])
```

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

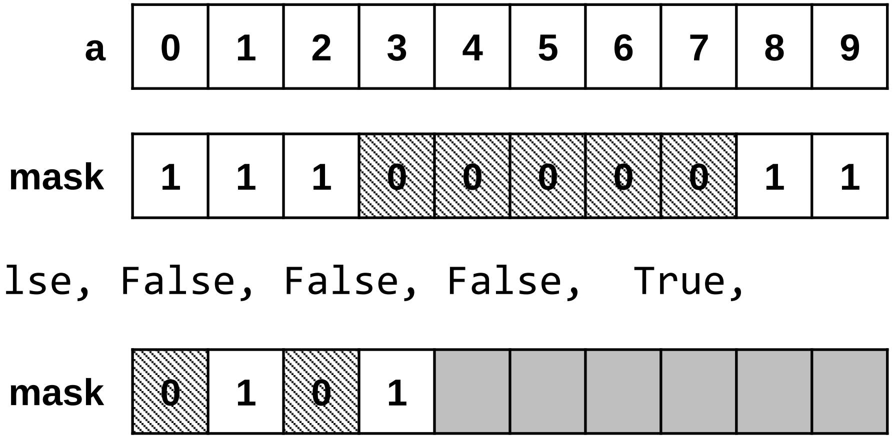
Slices Are References

- Slices are references to memory in the original array
- Changing values in a slice also changes the original array !

```
>>> a = np.arange(5)
>>> a
array([0, 1, 2, 3, 4])
>>> b = a[2:4]
>>> b
array([2, 3])
>>> b[0]=7
>>> a
array([0, 1, 7, 3, 4])
```

Masking

```
>>> a=np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
# creation of mask using ufunc
>>> mask=np.abs(a-5)>2
>>> mask
array([ True,  True,  True, False, False, False, False, False,  True,
True], dtype=bool)
>>> a[mask]
array([0, 1, 2, 8, 9])
>>> mask=np.array([0,1,0,1],dtype=bool)
# manual creation of mask
>>> mask
array([False,  True, False,  True], dtype=bool)
>>> a[mask]
array([1, 3])
```

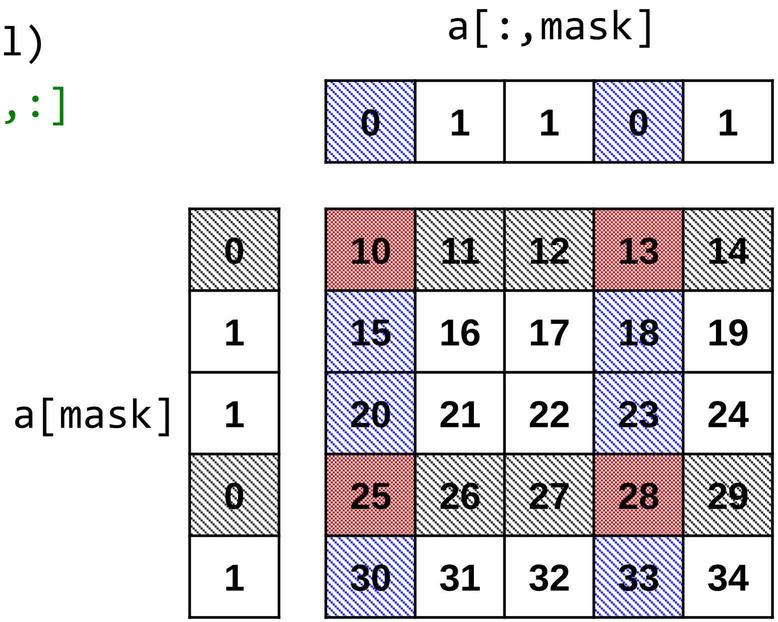


Masking and where

```
>>> a=np.arange(8)**2
>>> a
array([ 0,  1,  4,  9, 16, 25, 36, 49])
>>> mask=np.abs(a-9)>5
>>> mask
array([ True,  True, False, False,  True,  True,  True,  True],
dtype=bool)
# find the locations in array where expression is true
>>> np.where(mask)
(array([0, 1, 4, 5, 6, 7]),)
>>> loc=np.where(mask)
>>> a[loc]
array([ 0,  1, 16, 25, 36, 49])
```

Masking in 2D

```
>>> a=np.arange(25).reshape(5,5)+10
>>> a
array([[10, 11, 12, 13, 14],
       [15, 16, 17, 18, 19],
       [20, 21, 22, 23, 24],
       [25, 26, 27, 28, 29],
       [30, 31, 32, 33, 34]])
>>> mask=np.array([0,1,1,0,1],dtype=bool)
>>> a[mask]    # on rows, same as a[mask,:]
array([[15, 16, 17, 18, 19],
       [20, 21, 22, 23, 24],
       [30, 31, 32, 33, 34]])
>>> a[:,mask] # on columns
array([[11, 12, 14],
       [16, 17, 19],
       [21, 22, 24],
       [26, 27, 29],
       [31, 32, 34]])
```



Fancy Indexing - 1D

- **NumPy offers more indexing facilities than regular Python sequences.**
- **In addition to indexing by integers and slices, arrays can be indexed by arrays of integers and arrays of Booleans (as seen before).**

```
>>> a=np.arange(8)**2
>>> a
array([ 0,  1,  4,  9, 16, 25, 36, 49])
# indexing by position
>>> i=np.array([1,3,5,1])
>>> a[i]
array([ 1,  9, 25,  1])
>>> b=(np.arange(6)**2).reshape(2,-1)
>>> b
array([[ 0,  1,  4],
       [ 9, 16, 25]])
>>> i=[0,1,0]
>>> j=[0,2,1]
>>> b[i,j] # indexing 2D array by position
array([ 0, 25,  1])
```

Fancy Indexing - 2D

```
>>> b=(np.arange(12)**2).reshape(3,-1)
>>> b
array([[  0,   1,   4,   9],
       [ 16,  25,  36,  49],
       [ 64,  81, 100, 121]])
>>> i=[0,2,1]
>>> j=[0,2,3]
# indexing 2D array
>>> b[i,j]
array([  0, 100,  49])
# note the shape of the resulting array
>>> i=[[0,2],[2,1]]
>>> j=[[0,3],[3,1]]
# When an array of indices is used,
# the result has the same shape as the indices;
>>> b[i,j]
array([[  0, 121],
       [121,  25]])
```

idx	0	1	2	3
0	0	1	4	9
1	16	25	36	49
2	64	81	100	121

Scientific Computing with Python

Change RGB Image to Grayscale

Using Numpy to Process Image

- **RGB to Grayscale Conversion:**
  - Using simple average

$$V_{Gray} = \left(V_{Red} + V_{Green} + V_{Blue}\right)/3$$

  - Using weighted average (https://en.wikipedia.org/wiki/Grayscale)

$$V_{Gray} = 0.299V_{Red} + 0.587V_{Green} + 0.114V_{Blue}$$

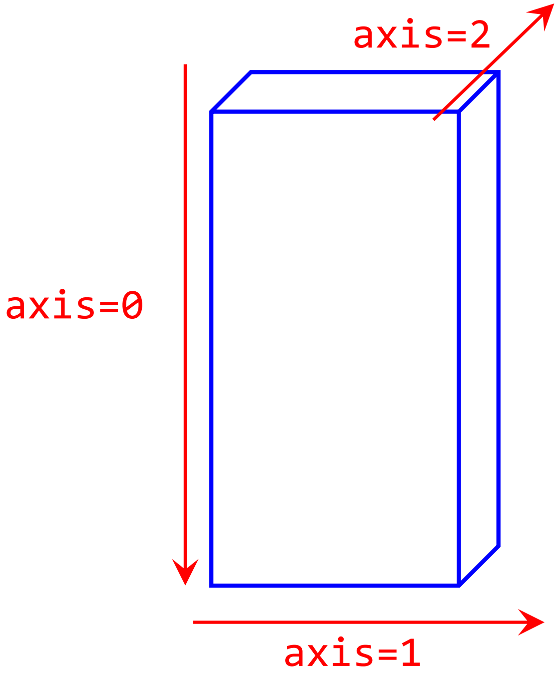
- **Loading and Displaying Images**

Load Image

```python
# import necessary images
import numpy as np
from scipy.misc import imread, imresize
import matplotlib.pyplot as plt
# To load an image, we use imread method from scipy's misc modules:
img = imread('cat.jpg')
print img.shape
```

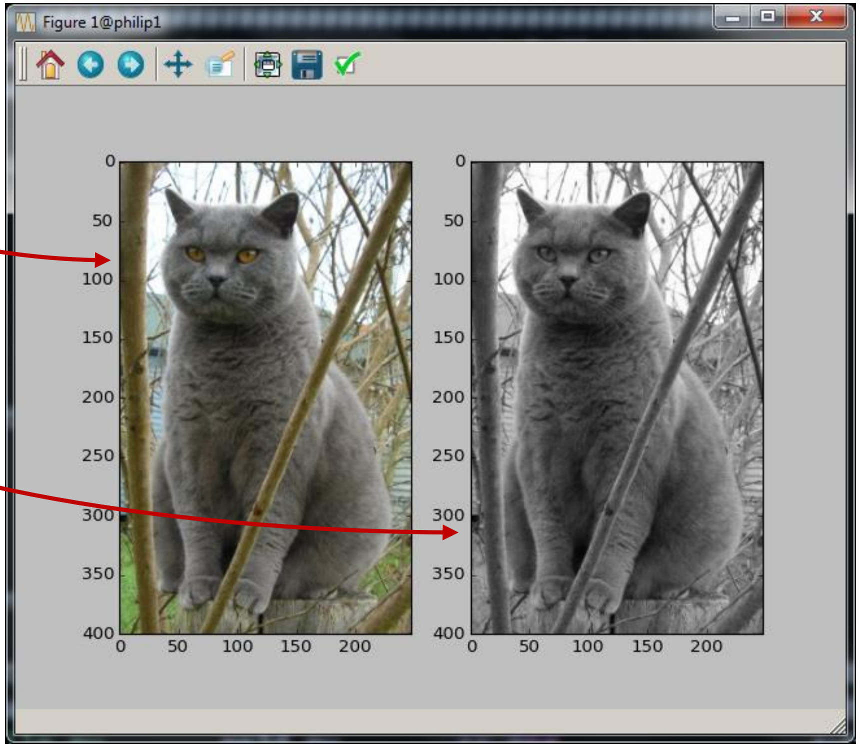
Shape of the loaded image in ipython:

```
In [2]: imread('cat.jpg')
Out[2]:
array([[[132, 128, 117],
        [155, 151, 139],
        [181, 175, 161],
        ...,
        [ 91,  76,  57],
        [ 89,  74,  55],
        [ 86,  71,  50]]], dtype=uint8)
```



Averaging The RGB Channel Values

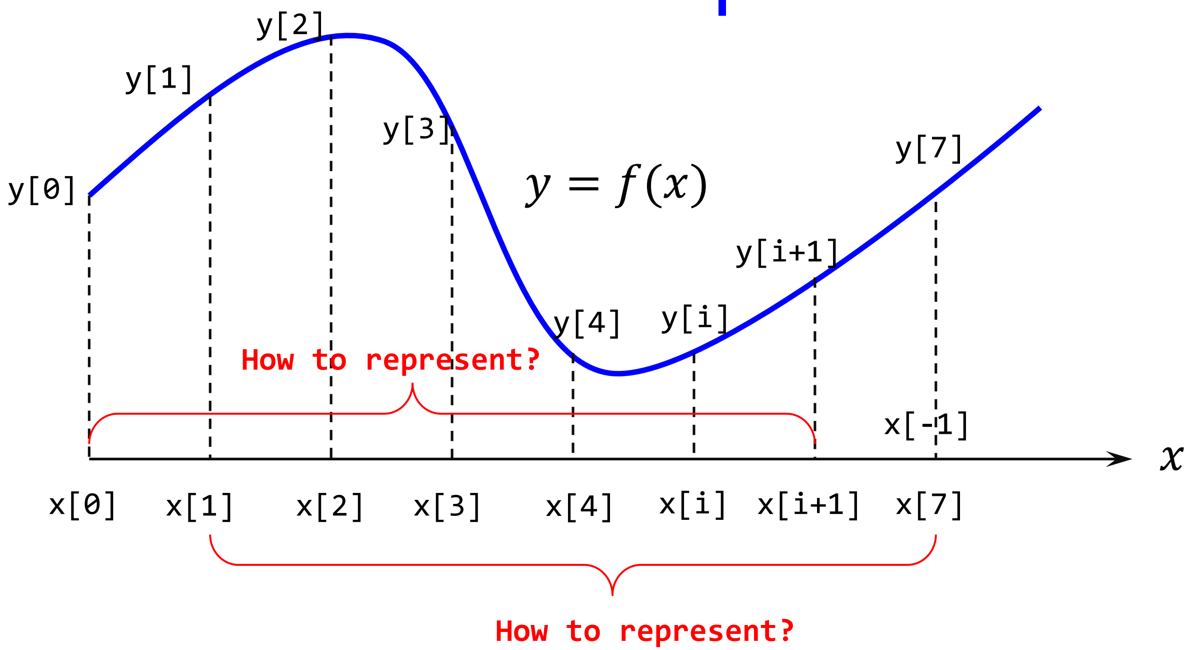
```
# This is simple average along axis=2
# img_tinted = np.average(img,axis=2)
# This is weighted average along axis=2
img_tinted = np.average(img,weights=[0.299,0.587,0.114],axis=2)
print img_tinted.shape
print img.shape
# plot the original image on the left
plt.subplot(1, 2, 1)
plt.imshow(img)
# plot the grayscale image on the left
plt.subplot(1, 2, 2)
plt.imshow(np.uint8(img_tinted),
    cmap='gray')
plt.show()
```



Scientific Computing with Python

Calculate Derivative

Problem Description



- **Numerical Derivative and Integration:**

$$y' = \frac{dy}{dx} \approx \frac{\Delta y}{\Delta x} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$

$$\int_a^b f(x)dx = \sum_{i=1}^{N} \frac{1}{2}(y_i + y_{i+1}) \cdot \Delta x$$

y[1]	y[2]	y[3]	y[4]

−

y[0]	y[1]	y[2]	y[3]

=

y[1]-y[0]	y[2]-y[1]	y[3]-y[2]	y[4]-y[3]

- **How to get a vector of Δy and Δx ?**

Calculate Derivative - Solution

- **Using Numpy slicing:**

```
import numpy as np
import matplotlib.pyplot as plt

# calculate the sin() function on evenly spaced data.
x = np.linspace(0,2*np.pi,101)
y = np.sin(x)

# use slicing to get dy and dx
dy=y[1:]-y[:-1]
dx=x[1:]-x[:-1]

dy_dx = dy/dx
```

Scientific Computing with Python

Introducing Scipy

Numerical Methods with Scipy

- **Scipy package (SCIentific PYthon) provides a multitude of numerical algorithms built on Numpy data structures**
- **Organized into subpackages covering different scientific computing areas**
- **A data-processing and prototyping environment almost rivaling MATLAB**

Major modules from scipy

- **Available sub-packages include:**
  - constants: physical constants and conversion factors
  - cluster: hierarchical clustering, vector quantization, K-means
  - integrate: numerical integration routines
  - interpolate: interpolation tools
  - io: data input and output
  - linalg: linear algebra routines
  - ndimage: various functions for multi-dimensional image processing
  - optimize: optimization algorithms including linear programming
  - signal: signal processing tools
  - sparse: sparse matrix and related algorithms
  - spatial: KD-trees, nearest neighbors, distance functions
  - special: special functions
  - stats: statistical functions
  - weave: tool for writing C/C++ code as Python multiline strings

Scipy Example: Integration

$$\int_1^3 x^2 dx = \frac{1}{3} x^3 \Big|_1^3$$

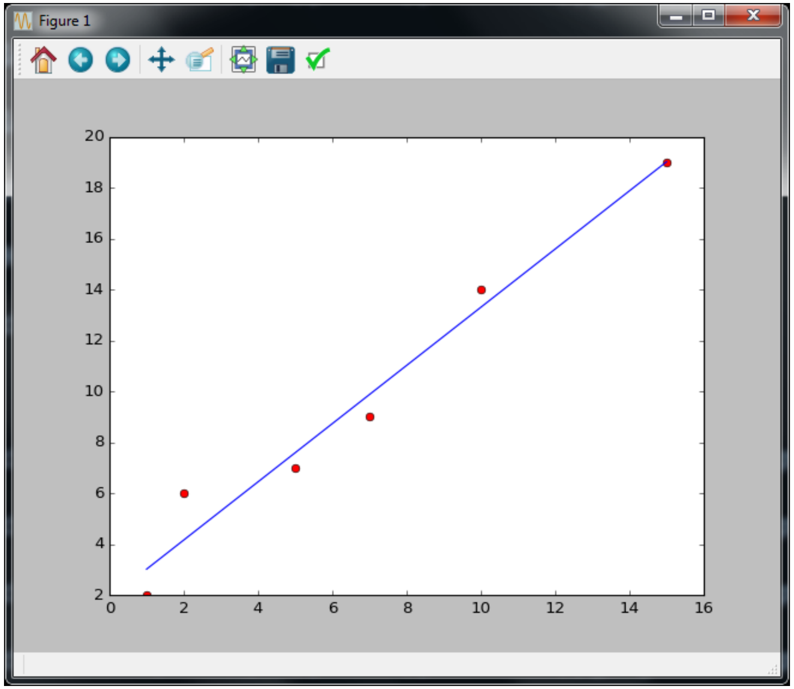
```
#!/usr/bin/env python
import scipy.integrate as integrate
import scipy.special as special
result_integ, err = integrate.quad(lambda x: x**2, 1, 3)
result_real = 1./3.*(3.**3-1**3)

print "result_real=", result_real
print "result_integ=", result_integ
```

Scipy Example: Regression

```python
#!/usr/bin/env python

from scipy import stats
import numpy as np
import matplotlib.pyplot as plt
```




```python
x = np.array([1, 2, 5, 7, 10, 15])
y = np.array([2, 6, 7, 9, 14, 19])
slope, intercept, r_value, p_value, std_err = stats.linregress(x,y)

plt.plot(x,y,'or')
yh = x*slope + intercept
plt.plot(x, yh, '-b')
plt.show()
```

Scientific Computing with Python

Mini-Project:
k Nearest Neighbor of images

Background

- **As our first approach, we will develop what we call a Nearest Neighbor Classifier to classify hand written digits dataset MNIST. This method will allow us to get an idea about the basic approach to an image classification problem.**

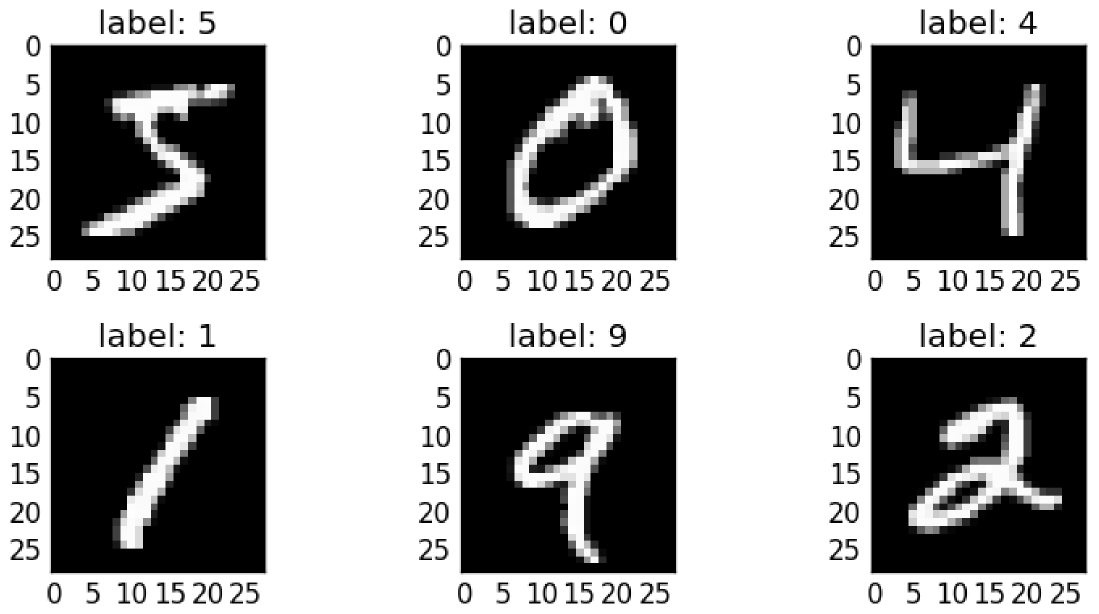
- **Example image classification dataset: MNIST.**
  - One popular toy image classification dataset is the MNIST dataset. This dataset consists of 60,000 tiny images that are 28 pixels high and wide.

- **Each image is labeled with one of 10 classes (0-9). These 60,000 images are partitioned into a training set of 50,000 images and a test set of 10,000 images.**

- **In the image below you can see 10 random example images from each one of the 10 classes:**

Introducing the MNIST problem

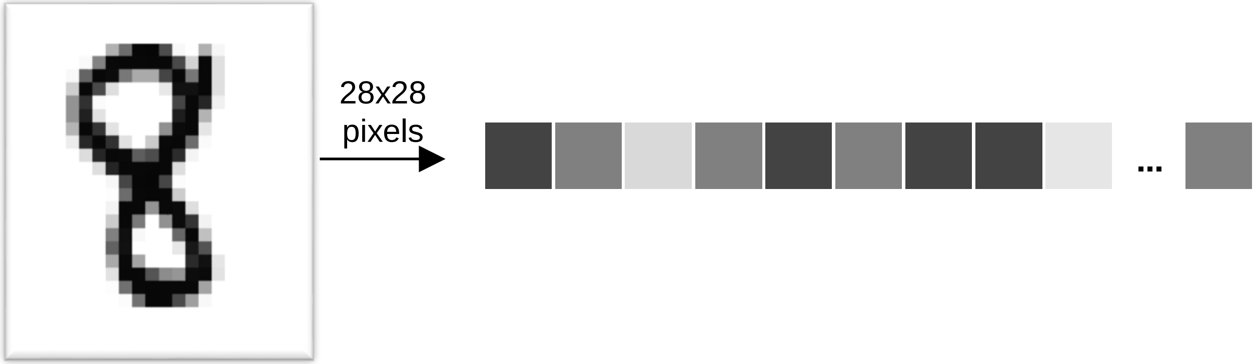
- **MNIST (Mixed National Institute of Standards and Technology database) is a large database of handwritten digits that is commonly used for training various image processing systems.**
- **It consists of images of handwritten digits like these:**



- **The MNIST database contains 50,000 training images, 10,000 validation images and 10,000 testing images.**

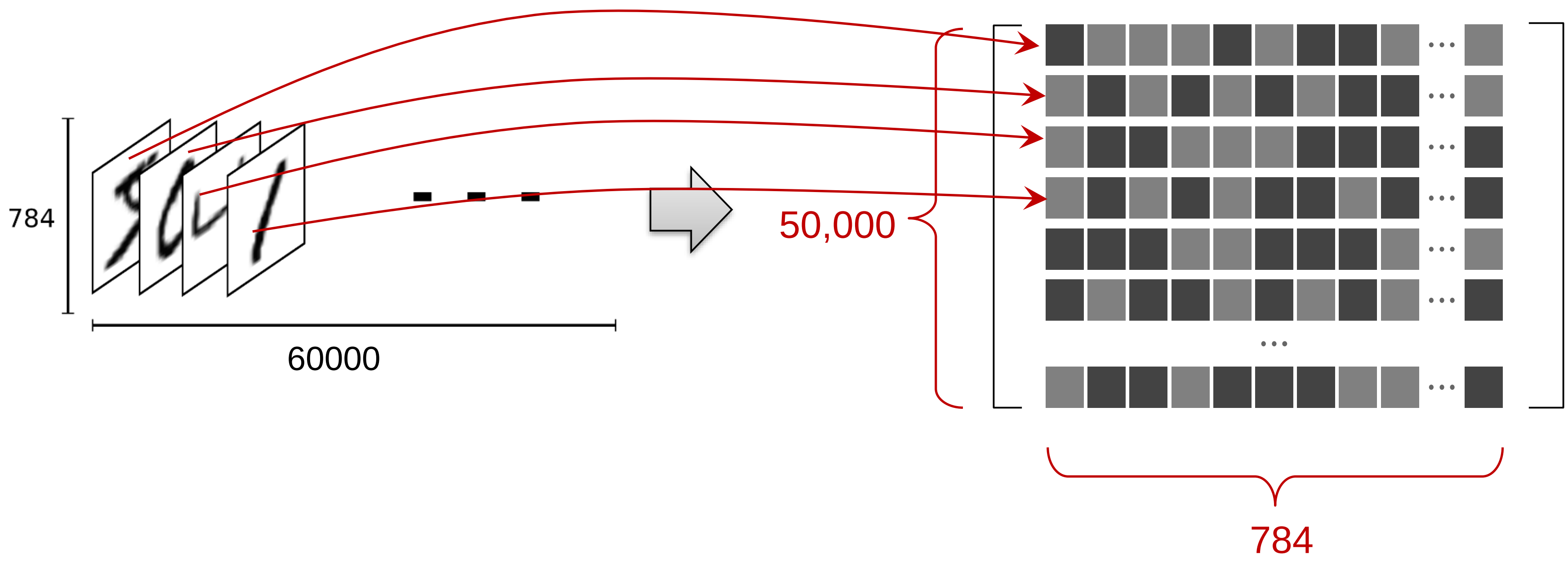
Flatten the 2D image into 1D vector

- We first flatten each image into a vector of 28x28 = 784 numbers. It doesn't matter how we flatten the array, as long as we're consistent between images.
- From this perspective, the MNIST images are just a bunch of points in a 784-dimensional vector space.



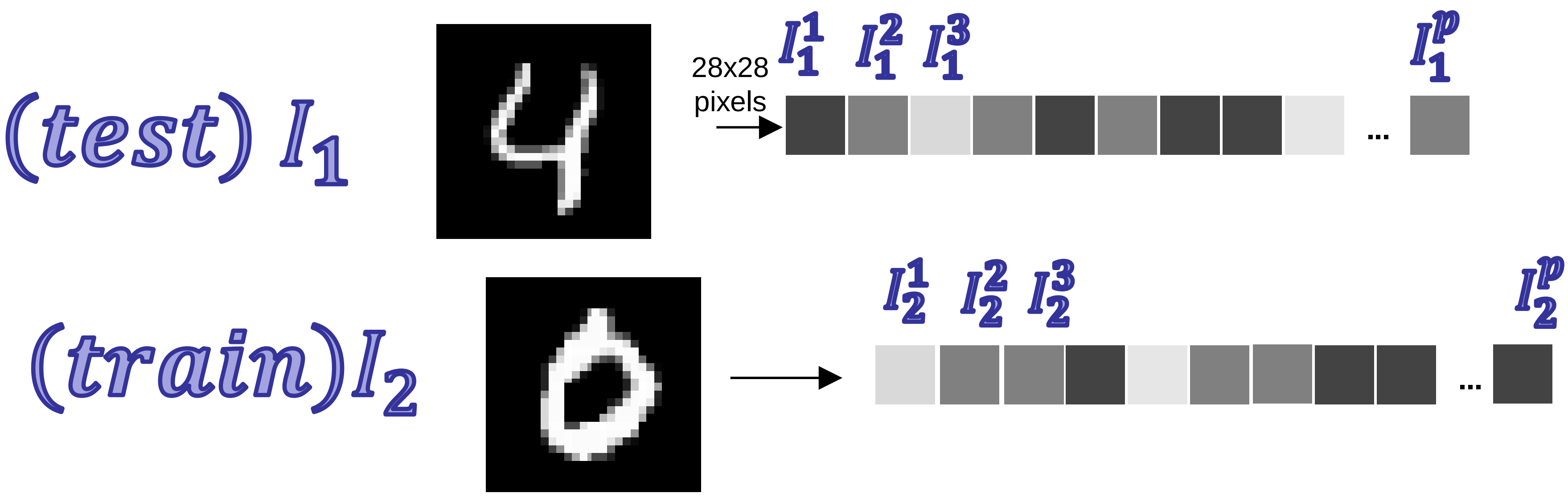
Result of the Flatten Operation

- **The result is that the training images is a matrix (tensor) with a shape of `[50000, 784]`.**
- **The first dimension is an index into the list of images and the second dimension is the index for each pixel in each image.**
- **Each entry in the tensor is a pixel intensity between 0 and 255, for a particular pixel in a particular image.**

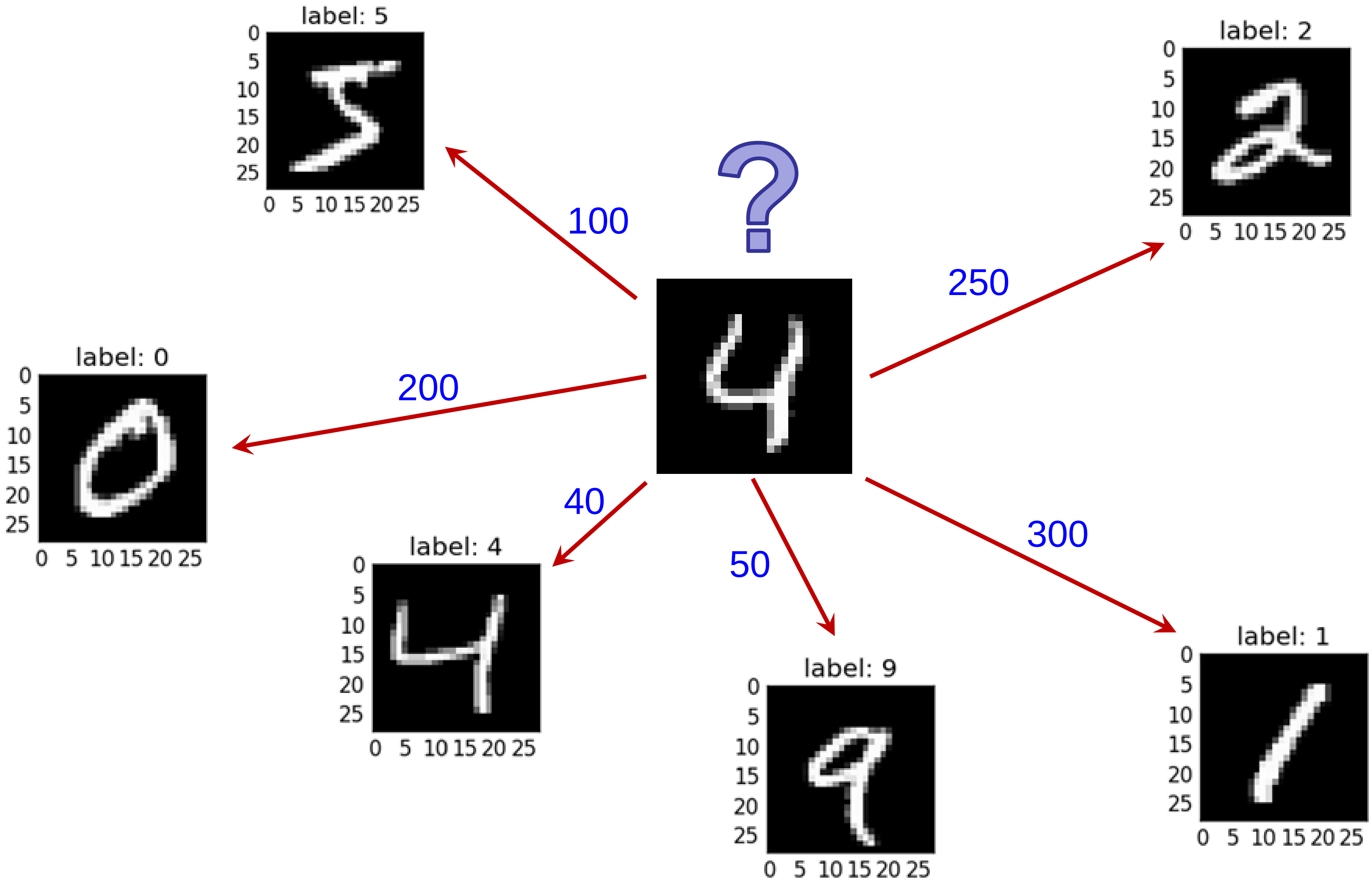


How kNN work for image classification?

- **For each test image, we "*compare*" the image with all the training set images, then we will find *k* nearest neighbor images and let the k images vote for the test image and determine the label of the test image.**
  - How do we compare image?
    - Use the L2 distance (Euclidean distance between two vectors):
    - $d_2(I_1, I_2) = \sqrt{(I_1^1 - I_2^1)^2 + (I_1^2 - I_2^2)^2 + \cdots + \left(I_1^p - I_2^p\right)^2} = \sqrt{\sum_{i=1}^{p}\left(I_1^i - I_2^i\right)^2}$

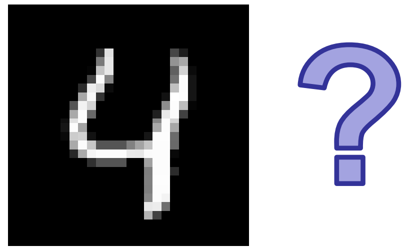


Visualization of K Nearest Neighbor



How do the k images vote the test image?

- **For example, given the below image that we need to label, we have found 7 nearest neighbors for this image:**



- **So based on the 7 neighbors, 4 votes “4”, 3 votes “9”, this image will be labeled as 4**