CS 5489 Machine Learning

Lecture 1b: Numpy, Matplotlib

Dr. Antoni B. Chan

Dept. of Computer Science, City University of Hong Kong

Outline

- 1. Python Intro
- 2. Python Basics (identifiers, types, operators)
- 3. Control structures (conditional and loops)
- 4. Functions, Classes
- 5. File IO, Pickle, pandas
- 6. NumPy
- 7. matplotlib
- 8. probability review

NumPy

- Library for multidimensional arrays and 2D matrices
- ndarray class for multidimensional arrays
 - elements are all the same type
 - aliased to array

```
In [1]:
         from numpy import * # import all classes from numpy
         a = arange(15)
Out[1]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14])
In [2]:
         b = a.reshape(3,5) # rows x columns
Out[2]:
         array([[ 0, 1,
                          2,
                              3,
                                   4],
                         7, 8,
                [ 5,
                     6,
                [10, 11, 12, 13, 14]])
In [3]:
                # get the shape (num rows x num columns)
```

```
Out[3]: (3, 5)
In [4]: b.ndim # get number of dimensions
Out[4]: 2
In [5]: b.size # get number of elements
Out[5]: 15
In [6]: b.dtype # get the element type
Out[6]: dtype('int64')
```

Array Creation

```
In [7]:
          a = array([1, 2, 3, 4])
                                    # use a list to initialize
 Out[7]: array([1, 2, 3, 4])
 In [8]:
          b = array([[1.1,2,3], [4,5,6]]) # or list of lists
 Out[8]:
          array([[1.1, 2., 3.],
                  [4., 5., 6.]
 In [9]:
           zeros((3,4)) # 3x4 array of zeros
 Out[9]:
          array([[0., 0., 0., 0.],
                  [0., 0., 0., 0.],
                  [0., 0., 0., 0.]])
In [10]:
          ones((2,4)) # 2x4 array of ones
Out[10]:
          array([[1., 1., 1., 1.],
                  [1., 1., 1., 1.]])
In [11]:
          full((3,4), 8.8) # 3x4 array with all 8.8
Out[11]: array([[8.8, 8.8, 8.8, 8.8],
                  [8.8, 8.8, 8.8, 8.8],
                  [8.8, 8.8, 8.8, 8.8]])
In [12]:
          empty( (2,3) ) # create an array, but do not prepopulate it.
                         # contents are random
Out[12]: array([[1.1, 2., 3.],
```

[4., 5., 6.]

```
In [13]:
           arange(0,5,0.5) # from 0 to 5 (exclusive), increment by 0.5
           array([0., 0.5, 1., 1.5, 2., 2.5, 3., 3.5, 4., 4.5])
Out[13]:
In [14]:
           linspace(0,1,10) # 10 evenly-spaced numbers between 0 to 1 (inclusive)
                            , 0.11111111, 0.22222222, 0.33333333, 0.44444444,
Out[14]:
           array([0.
                  0.5555556, 0.66666667, 0.77777778, 0.88888889, 1.
In [15]:
          logspace(-3,3,13) # 13 numbers evenly spaced in log-space between 1e-3 and 1e3
          array([1.0000000e-03, 3.16227766e-03, 1.0000000e-02, 3.16227766e-
Out[15]:
                  1.00000000e-01, 3.16227766e-01, 1.00000000e+00, 3.16227766e+
           00,
                  1.00000000e+01, 3.16227766e+01, 1.00000000e+02, 3.16227766e+
           02,
                  1.00000000e+031)
```

Array Indexing

• One-dimensional arrays are indexed, sliced, and iterated similar to Python lists.

```
In [16]:
            a = array([1,2,3,4,5])
            a[2]
Out[16]:
In [17]:
                             # index 2 through 4
            a[2:5]
Out[17]:
            array([3, 4, 5])
In [18]:
            a[0:5:2]
                            # index 0 through 4, by 2
Out[18]:
            array([1, 3, 5])
In [19]:
            # iterating with loop
            for i in a:
               print(i)
            1
            2
            3
            4
            5
```

For multi-dimensional arrays, each axis had an index.

indices are given using tuples (separated by commas)

```
In [20]:
           a = array([[1, 2, 3], [4, 5, 6], [7,8,9]])
           print(a)
            [[1 2 3]
            [4 5 6]
             [7 8 9]]
In [21]:
           a[0,1]
                   # row 0, column 1
Out[21]:
In [22]:
                    # all elements in column 1
           a[:,1]
Out[22]: array([2, 5, 8])
In [23]:
           a[0:2, 1:3] # sub array: rows 0-1, and columns 1-2
Out[23]: array([[2, 3],
                   [5, 6]])
In [24]:
           # "for" iterates over the first index (rows)
           for r in a:
               print("--")
               print(r)
           [1 2 3]
           [4 5 6]
           [7 8 9]
            • indexing with a boolean mask
In [25]:
           a = array([3, 1, 2, 4])
           m = array([True, False, False, True])
           print("m =", m)
                           # select with a mask
           m = [ True False False True]
Out[25]: array([3, 4])
```

multi-dimensional arrays (tensors)

- 3 x 2 x 4 tensor
 - prints as three 2x4 arrays
 - last index is iterated first

```
In [26]:
           a = arange(24)
           b = a.reshape((3,2,4))
           print(b)
           [[[ 0 1 2 3]
             [ 4 5 6 7]]
            [[ 8 9 10 11]
             [12 13 14 15]]
            [[16 17 18 19]
             [20 21 22 23]]]
           • indexing is similar to 2-dim arrays (i,j,k)
In [27]:
           b[2,0,1]
Out[27]:
           17
           • extract a "slice"
In [28]:
           b[1,:] # i=1
           array([[ 8, 9, 10, 11],
Out[28]:
                  [12, 13, 14, 15]])
In [29]:
           b[:,1,:] # j=1
Out[29]: array([[ 4, 5, 6, 7],
                  [12, 13, 14, 15],
                  [20, 21, 22, 23]])
In [30]:
           b[:,:,1] # k=1
Out[30]: array([[ 1, 5],
                   [ 9, 13],
                  [17, 21]])
In [31]:
           # iterate over the first index
           for s in b:
              print("--")
              print(s)
           [[0 1 2 3]
            [4 5 6 7]]
           [[ 8 9 10 11]
            [12 13 14 15]]
           [[16 17 18 19]
            [20 21 22 23]]
```

Array Shape Manipulation

• The shape of an array can be changed

```
In [32]:
           a = array([[1,2,3], [4, 5, 6]])
           print(a)
           a.shape
            [[1 2 3]
            [4 5 6]]
Out[32]:
           (2, 3)
In [33]:
           a.ravel()
                         # return flattened array (last index iterated first).
Out[33]:
           array([1, 2, 3, 4, 5, 6])
In [34]:
           a.transpose() # return transposed array (swap rows and columns)
Out[34]:
           array([[1, 4],
                   [2, 5],
                   [3, 6]])
In [35]:
           a.reshape(3,2) # return reshaped array
Out[35]: array([[1, 2],
                   [3, 4],
                   [5, 6]])
In [36]:
           a.resize(3,2) # change the shape directly (modifies a)
           print(a)
            [[1 2]
            [3 4]
            [5 6]]
```

Concatenating arrays

```
In [39]: r_[a,b] # concatenate as row vectors
Out[39]: array([1, 2, 3, 4, 5, 6])
```

Stacking arrays

Array Operations

• operators are applied **elementwise**

```
In [42]:
           a = array([20,30,40,50])
           b = arange( 4 ) # [0 1 2 3]
                           # element-wise subtraction
Out[42]: array([20, 29, 38, 47])
In [43]:
                           # element-wise exponentiation
Out[43]:
           array([0, 1, 4, 9])
In [44]:
           10*sin(a)
                          # element-wise product and sin
Out[44]: array([ 9.12945251, -9.88031624, 7.4511316 , -2.62374854])
In [45]:
           a < 35
                           # element-wise comparison
Out[45]: array([ True, True, False, False])
           • product operator (*) is elementwise
               • i.e., Hadamard product
```

```
A = array([[1,1],
                     [0,1]])
           B = array([[2,0],
                      [3,4]])
           A*B
                                    # elementwise product
Out[46]: array([[2, 0],
                  [0, 4]])
           • compound assignment: *= , += , -=

    unary operators

In [47]:
           a = array([[1,2,3], [4, 5, 6]])
           a.sum()
Out[47]:
           21
In [48]:
           a.min()
Out[48]:
In [49]:
           a.max()
Out[49]:

    unary operators on each axis of array

In [50]:
           a = array([[1,2,3], [4, 5, 6]])
           a.sum(axis=0) # sum over rows
Out[50]:
          array([5, 7, 9])
In [51]:
           a.sum(axis=1)
                         # sum over column
Out[51]:
           array([ 6, 15])
           • Numpy provides functions for other operations (called universal functions)
               argmax, argmin, min, max
               average, cov, std, mean, median,
               ceil, floor
               cumsum, cumprod, diff, sum, prod
               inv, dot, trace, transpose
```

Broadcasting

any binary operators (+, -, *, etc)

• if the two operands are not the same size

- broadcasting tries to extend the singleton dimensions of one operand to match the other operand.
- an Error is thrown if two operands can't be broadcast together.
- operands do not need to have the same number of dimensions
 - match dimensions from the right

- a and b are not the same dimensions,
 - b is "stretched" so that it fills in a 2x3 shape

```
a: 2 x 3
b: 3
result: 2 x 3
```

```
In [54]: a + b
Out[54]: array([[2, 4, 6],
```

[5, 7, 9]])

• c is stretched so that it fills in a 2x3 shape

```
a: 2 x 3
c: 2 x 1
result: 2 x 3
```

```
In [56]: a+c
```

```
Out[56]: array([[2, 3, 4], [6, 7, 8]])
```

b and c are both stretched to 2x3 shape

```
b: 3
c: 2 x 1
result: 2 x 3
```

```
In [57]: b+c
Out[57]: array([[2, 3, 4],
```

[3, 4, 5]])

• "newaxis" can insert an extra dimension

```
b: 3
b[:,newaxis]: 3 x 1
result: 3 x 3
```

Brief Linear Algebra Review

· column vector:

$$\mathbf{x} = egin{bmatrix} x_1 \ dots \ x_d \end{bmatrix} \in \mathbb{R}^d$$

• matrix:

$$\mathbf{A} = egin{bmatrix} a_{1,1} & \cdots & a_{1,n} \ dots & \ddots & dots \ a_{m,1} & \cdots & a_{m,n} \end{bmatrix} \in \mathbb{R}^{m imes n}$$

- matrix as collection of column vectors: $\mathbf{A} = egin{bmatrix} |&&&&|\\ \mathbf{a}_1&\cdots&\mathbf{a}_n\\ |&&&| \end{bmatrix}$
 - \mathbf{a}_i is the i-th column of \mathbf{A} .

Transpose: swap rows and columns

$$\mathbf{x}^T = [x_1 \cdots x_d]$$

```
In [61]: z = x.transpose()
print(z)
```

[[1 2 3]]

Inner product

- Inner product: $\mathbf{x}^T\mathbf{y} = \sum_{i=1}^d x_i y_i$
 - measures the similarity between vectors \mathbf{x} and \mathbf{y} .

```
In [62]: x = array([1, 2, 3])
y = array([2, 1, 1])
inner(x,y)
```

Out[62]: 7

• Length (norm):

$$||\mathbf{x}|| = \sqrt{\mathbf{x}^T\mathbf{x}} = \sqrt{\sum_{i=1}^d x_i^2}$$

```
In [63]: x = array([1, 2, 3])
    linalg.norm(x)
```

Out[63]: 3.7416573867739413

• Distance between two vectors:

$$||\mathbf{x}-\mathbf{y}|| = \sqrt{\sum_{i=1}^d (x_i-y_i)^2}$$

```
In [64]: y = array([2, 1, 1])
    linalg.norm(x-y)
```

Out[64]: 2.449489742783178

ullet Outerproduct between two vectors: $\mathbf{x}\mathbf{y}^T = [\ y_1\mathbf{x} \ \cdots \ y_d\mathbf{x}\]$

$$\mathbf{x}\mathbf{y}^T = egin{bmatrix} x_1y_1 & \cdots & x_1y_d \ dots & \ddots & dots \ x_dy_1 & \cdots & x_dy_d \end{bmatrix}$$

Matrix multiplication

• need compatible dimensions: $\mathbf{C}_{m \times n} = \mathbf{A}_{m \times d} \mathbf{B}_{d \times n}$

$$\mathbf{A} = egin{bmatrix} egin{bmatrix} a_{1,1} & \cdots & a_{1,n} \ dots & \ddots & dots \ a_{m,1} & \cdots & a_{m,n} \end{bmatrix}, \quad \mathbf{B} = egin{bmatrix} egin{bmatrix} b_{1,1} & \cdots & b_{1,n} \ dots \ b_{m,1} & \cdots & dots \ \end{pmatrix}$$

• Entry in **C**:

$$c_{i,j} = \mathbf{a}_i \mathbf{b}_j = \sum_{k=1}^d a_{i,d} b_{d,j}$$

```
Out[66]: array([[ 2, 3], [-2, 3]])
```

Matrix-Vector multiplication

- Different interpretations if using transpose or not.
- Ax: Linear combination of the columns of A
 - ullet $\mathbf{A} \in \mathbb{R}^{m imes d}, \mathbf{x} \in \mathbb{R}^d$:

$$\mathbf{y} = \mathbf{A}\mathbf{x} = egin{bmatrix} | & & | \ \mathbf{a}_1 & \cdots & \mathbf{a}_d \ | & & | \end{bmatrix} egin{bmatrix} x_1 \ dots \ x_d \end{bmatrix} = \sum_{i=1}^d x_i \mathbf{a}_i \in \mathbb{R}^m$$

```
x = array([-1, 1])
A @ x # matrix multiplicattion
```

```
Out[67]: array([1, 2])
```

• $\mathbf{A}^T \mathbf{x}$: Vector of inner products with columns of \mathbf{A}

•
$$\mathbf{A} \in \mathbb{R}^{d \times m}, \mathbf{x} \in \mathbb{R}^d$$
:

Out[68]: array([2, 3])

Matrix-matrix multiplication

AB: A multiplied by each column of B

$$\mathbf{A}\mathbf{B} = \mathbf{A} egin{bmatrix} | & & & | \ \mathbf{b}_1 & \cdots & \mathbf{b}_n \ | & & | \end{bmatrix} = egin{bmatrix} | & \mathbf{A}\mathbf{b}_1 & \cdots & \mathbf{A}\mathbf{b}_n \ | & & | \end{bmatrix}$$

• $\mathbf{A}^T\mathbf{B}$: matrix of inner products between columns of \mathbf{A} and \mathbf{B}

$$\mathbf{A}^T \mathbf{B} = \mathbf{A}^T \begin{bmatrix} | & & | \\ \mathbf{b_1} & \cdots & \mathbf{b_n} \\ | & & | \end{bmatrix} = \begin{bmatrix} \mathbf{a_1}^T \mathbf{b_1} & \cdots & \mathbf{a_1}^T \mathbf{b_n} \\ \vdots & \ddots & \vdots \\ \mathbf{a_m}^T \mathbf{b_1} & \cdots & \mathbf{a_m}^T \mathbf{b_n} \end{bmatrix} = \begin{bmatrix} \mathbf{a_i}^T \mathbf{b_j} \end{bmatrix}_{ij}$$

Out[70]: array([[-1, 3], [-2, 3]])

- $\mathbf{A}\mathbf{B}^T$: sum of outer products of between columns of \mathbf{A} and \mathbf{B}

$$\mathbf{A}\mathbf{B}^T = egin{bmatrix} |&&&&|\ \mathbf{a}_1&\cdots&\mathbf{a}_n\ |&&&&| \end{bmatrix} egin{bmatrix} -&&\mathbf{b}_1^T&-\ &dots\ -&&\mathbf{b}_n^T&- \end{bmatrix} = \sum_{i=1}^n \mathbf{a}_i \mathbf{b}_i^T$$

Copies and Views

- When operating on arrays, data is sometimes copied and sometimes not.
- No copy is made for simple assignment.
 - Be careful!

- View or shallow copy
 - different array objects can share the same data (called a view)
 - happens when slicing

```
In [74]: c = a.view() # create a view of a
```

```
c is a
                          # not the same object
Out[74]:
           False
In [75]:
                         # but the data is owned by a
           c.base is a
Out[75]:
           True
In [76]:
           c.shape = 2,2 # change shape of c
Out[76]:
           array([[ 1, -2],
                   [ 3, 4]])
In [77]:
                           # but the shape of a is the same
Out[77]:
           array([ 1, -2,
                             3,
                                  41)

    Deep copy

In [78]:
                               # create a complete copy of a (new data is created)
           d = a.copy()
                               # not the same object
Out[78]:
           False
In [79]:
           d.base is a
                              # not sharing the same data
Out[79]:
           False
```

Outline

- 1. Python Intro
- 2. Python Basics (identifiers, types, operators)
- 3. Control structures (conditional and loops)
- 4. Functions, Classes
- 5. File IO, Pickle, pandas
- 6. NumPy
- 7. matplotlib
- 8. probability review

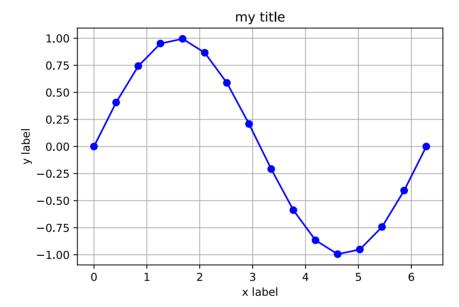
Visualizing Data

- Use matplotlib package to make plots and graphs
- Works with Jupyter to show plots within the notebook

```
In [80]: # setup matplotlib
%matplotlib inline
# setup output image format (Chrome works best)
import IPython.core.display
IPython.core.display.set_matplotlib_formats("svg") # file format
import matplotlib.pyplot as plt
```

- Each cell will start a new figure automatically.
- Plots are made piece by piece.

```
In [81]: x = linspace(0,2*pi,16)
y = sin(x)
plt.plot(x, y, 'bo-')
plt.grid(True)
plt.ylabel('y label'); plt.xlabel('x label'); plt.title('my title')
plt.show()
```



- plot string specifies three things (e.g., 'bo-')
 - colors:
 - blue, red, green, magenta, cyan, yellow, black, white
 - markers:
 - ∘ "" point; "o" circle
 - "v" triangle down; "^" triangle up
 - ∘ "<" triangle left; ">" triangle right
 - ∘ "8" octagon; "s" square
 - ∘ "p" pentagon "*" star
 - "h" hexagon1
 - "+" plus; "x" x
 - o "d" thin_diamond
 - line styles:
 - ∘ '-' solid line

- ∘ '--' dashed line
- ∘ '-.' dash-dotted line
- ':' dotted lione

Outline

- 1. Python Intro
- 2. Python Basics (identifiers, types, operators)
- 3. Control structures (conditional and loops)
- 4. Functions, Classes
- 5. File IO, Pickle, pandas
- 6. NumPy
- 7. matplotlib
- 8. probability review

Brief Review of Probability

- Random variable (r.v.) X takes a value in \mathcal{X} (set of possible values) at random.
- Associated with a probability distribution p(X) that describes the frequency of outcomes of the X.

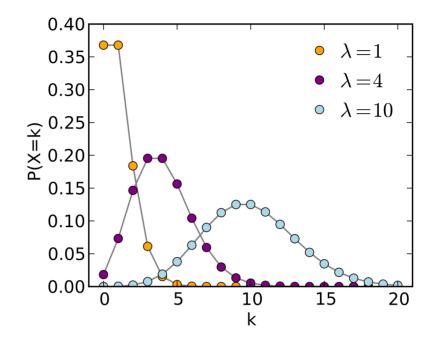
Discrete random variables

- Probability mass function (pmf)
- ullet p(X=x) is the probability of r.v. X taking value x
 - we will use simpler notation p(x)
- properties
 - $0 \le p(x) \le 1$
 - $\sum_{x \in \mathcal{X}} p(x) = 1$ \Rightarrow "normalized to 1"
- Example: Bernoulli (coin flip)
 - $\mathcal{X} = \{0, 1\}$
 - probability mass function (pmf)
 - $\circ \ p(x=1) = \pi$ \Rightarrow "probability of 1 occurring"
 - $\circ \ p(x=0) = 1 \pi$ \Rightarrow "probability of 0 occurring"
 - \circ combined: $p(x) = \pi^x (1-\pi)^{1-x}$
- Example: Poisson

 number of arrivals over a fixed time period (e.g., number of phone calls in a fixed interval)

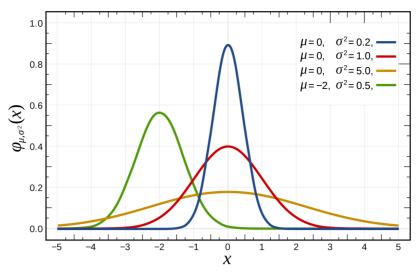
- $\mathcal{X} = \{0, 1, 2, \cdots\}$
- λ = average arrival rate ($\lambda > 0$)
- probability mass function

$$p(x) = \frac{1}{x!}e^{-\lambda}\lambda^x$$



Continuous random variables

- probability density function (pdf).
- p(x) is the likelihood of x.
- properties:
 - $0 \le p(x) \Rightarrow$ non-negative probability
 - $\int p(x)dx=1$, \Rightarrow "normalized to 1"
 - $p(a \leq x \leq b) = \int_a^b p(x) dx$ \Rightarrow "probability of x between [a,b]"
- Example: Gaussian (Normal)
 - ullet $\mathcal{X}=\mathbb{R}$ (real numbers)
 - μ =mean, σ^2 = variance
 - $\circ \ \sigma$ = standard deviation ("the spread of the values")
 - pdf: $p(x)=rac{1}{\sqrt{2\pi\sigma^2}}e^{-rac{1}{2\sigma^2}(x-\mu)^2}$



Joint probability

- Distribution of more than one r.v.
 - p(X=x,Y=y) probability that X=x **and** Y=y. \circ simpler notation p(x,y).
- Example:
 - joint probability table (sums to 1)

p(x,y)	Y=0	Y=1
X=0	0.08	0.12
X=1	0.32	0.48

Marginal probability

- Distribution over one r.v. of the joint distribution
- · Obtained by summing over the other r.v.
 - \bullet Discrete: $p(x) = \sum_{y \in \mathcal{Y}} p(x,y)$
 - ullet Continuous: $p(x)=\int p(x,y)dy$
- Example:

p(x,y)	Y=0	Y=1	p(x)
X=0	0.08	0.12	0.20
X=1	0.32	0.48	0.80
p(y)	0.40	0.60	

Conditional probability

- Distribution of one r.v. when the value of another r.v. is known (given).
 - $p(x|y) = \frac{p(x,y)}{p(y)}$
 - the value *y* is "given".

• Example:

•
$$p(x=0|y=0) = \frac{p(x=0,y=0)}{p(y=0)} = \frac{0.08}{0.4} = 0.2$$

• $p(x=1|y=0) = \frac{p(x=1,y=0)}{p(y=0)} = \frac{0.32}{0.4} = 0.8$

$$p(x=1|y=0) = rac{p(x=1,y=0)}{p(y=0)} = rac{0.32}{0.4} = 0.8$$

• p(x|y=0) is a distribution over x, so sums to 1.

Bayes' Rule

- joint probabability can be rewritten as:
 - p(x,y) = p(x|y)p(y)
 - p(x,y) = p(y|x)p(x)
- · Thus.
 - p(y|x)p(x) = p(x|y)p(y)
 - $lack p(y|x) = rac{p(x|y)p(y)}{p(x)}$
- Looking at denominator...
 - marginalize: $p(x) = \int p(x,y)dy$
 - ullet use conditional probability: $p(x) = \int p(x|y) p(y) dy$
- · Baves' Rule
 - $p(y|x) = \frac{p(x|y)p(y)}{\int p(x|y)p(y)dy}$
 - ullet Given only p(x|y) and p(y), we can "invert" the conditioning to obtain p(y|x).
- We will use this next week to build a classifier using probability distributions.

Python Tutorials

- Python https://docs.python.org/3/tutorial/
- numpy https://docs.scipy.org/doc/numpy-dev/user/quickstart.html
- "Machine Learning in Action" Appendix A, Ch. 1
- scikit-learn http://scikit-learn.org/stable/tutorial/
- matplotlib http://matplotlib.org/users/pyplot_tutorial.html
- pandas https://pandas.pydata.org/pandas-docs/stable/tutorials.html