CS 5489 Machine Learning

Lecture 1b: Numpy, Matplotlib

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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 \times columns
        b
Out[2]: array([[ 0, 1,
               [5, 6, 7, 8, 9],
               [10, 11, 12, 13, 14]])
In [3]: b.shape # 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
Out[13]: array([0., 0.5, 1., 1.5, 2., 2.5, 3., 3.5, 4., 4.5])
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
Out[15]: array([1.00000000e-03, 3.16227766e-03, 1.00000000e-02, 3.16227766e-02,
                 1.00000000e-01, 3.16227766e-01, 1.00000000e+00, 3.16227766e+00, 1.00000000e+01, 3.16227766e+01, 1.0000000e+02, 3.16227766e+02,
                 1.00000000e+03])
```

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]: 3
In [17]: a[2:5] # index 2 through 4
```

```
Out[17]: array([3, 4, 5])
                   # index 0 through 4, by 2
In [18]: a[0:5:2]
Out[18]: array([1, 3, 5])
In [19]: # iterating with loop
         for i in a:
             print(i)
          1
          2
          3
          • 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]: 2
In [22]: a[:,1]
                 # all elements in column 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)

```
    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
Out[28]: array([[ 8, 9, 10, 11],
                 [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
[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
```

prints as three 2x4 arrays

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
```

Stacking arrays

Array Operations

```
In [42]: a = array( [20,30,40,50] )
         b = arange( 4 ) # [0 1 2 3]
                            # element-wise subtraction
         a - b
Out[42]: array([20, 29, 38, 47])
In [43]: b**2
                            # 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
In [46]: 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]: 1
In [49]: a.max()
Out[49]: 6

    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

 $b[:,newaxis]: 3 \times 1$

3 x 3

[3, 4, 5],

result:

In [58]: b + b[:,newaxis]

Out[58]: array([[2, 3, 4],

- 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
In [52]: a = array( [[1,2,3],
                        [4,5,6]])
In [53]: b = array([1,2,3])
            • 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
                  2 x 3
                 2 x 1
          result: 2 x 3
In [55]: c = array([[1],
                        [2]])
In [56]: a+c
Out[56]: array([[2, 3, 4],
                   [6, 7, 8]])
            • b and c are both stretched to 2x3 shape
                  2 x 1
          c:
          result: 2 x 3
In [57]: b+c
Out[57]: array([[2, 3, 4],
                   [3, 4, 5]])
            • "newaxis" can insert an extra dimension
```

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} .

Inner product

[[1 2 3]]

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

```
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

• Outerproduct between two vectors: $\mathbf{x}\mathbf{y}^T = [\ y_1\mathbf{x} \quad \cdots \quad 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: $\mathbf{C}_{m \times n} = \mathbf{A}_{m \times d} \mathbf{B}_{d \times n}$

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

• Entry in C:

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

Matrix-Vector multiplication

• Different interpretations if using transpose or not.

- Ax: Linear combination of the columns of A
 - $\mathbf{A} \in \mathbb{R}^{m \times d}$, $\mathbf{x} \in \mathbb{R}^d$:

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

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

- $\mathbf{A}^T \mathbf{x}$: Vector of inner products with columns of \mathbf{A}
 - $oldsymbol{A} \in \mathbb{R}^{d imes m}, oldsymbol{\mathbf{x}} \in \mathbb{R}^d$:

$$\mathbf{y} = \mathbf{A}^T \mathbf{x} = egin{bmatrix} | & & | & | & | \\ \mathbf{a}_1 & \cdots & \mathbf{a}_d & | & \mathbf{x} \\ | & & | & | & \end{bmatrix}^T \mathbf{x}$$
 $= egin{bmatrix} - & \mathbf{a}_1^T & - & | & \mathbf{a}_1^T \mathbf{x} \\ & dots & | & | & \mathbf{x} = \begin{bmatrix} \mathbf{a}_1^T \mathbf{x} \\ dots & | & | & | \\ \mathbf{a}_m^T \mathbf{x} \end{bmatrix} \in \mathbb{R}^m$

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

Matrix-matrix multiplication

• AB: A multiplied by each column of B

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

Out[69]: array([[-1, 3], [-2, 3]])

- $\mathbf{A}^T\mathbf{B}$: 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]]
            • AB^T: sum of outer products of between columns of A and B $$\mathbf{A}\mathbf{B}^T = \left[
                                                           \mathbf{a}_1 \quad \cdots \quad \mathbf{a}_n
              \right] \left[
              \left| \right| = \sum_{i=1}^n \mathbb{a}_i \mathbb{b}_i^T
          $$
In [71]: A = array([[1, 2],
                       [2, 1]])
          B = array([[-1,1],
                       [0, 1]])
          A @ B.transpose()
Out[71]: array([[ 1, 2],
                    [-1, 1]])
          Copies and Views
            • When operating on arrays, data is sometimes copied and sometimes not.
            • No copy is made for simple assignment.
                ■ Be careful!
In [72]: a = array([1,2,3,4])
                                 # simple assignment (no copy made!)
          b is a
                                 # yes, b references the same object
Out[72]: True
```

```
In [72]: a = array([1,2,3,4])
b = a  # simple assignment (no copy made!)
b is a  # yes, b references the same object

Out[72]: True

In [73]: b[1] = -2  # changing b also changes a
a  array([1, -2, 3, 4])

• 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]: c.base is a  # but the data is owned by a
```

Out[75]: True

In [76]: c.shape = 2,2 # change shape of c

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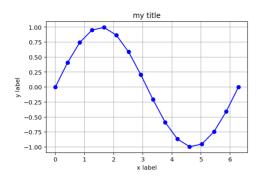
Visualizing Data

- 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 matplotlib_inline # setup output image format
matplotlib_inline.backend_inline.set_matplotlib_formats('retina')
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:
 - o blue, red, green, magenta, cyan, yellow, black, white
 - markers:
 - o '.' point; 'o' circle
 - '+' plus; 'x' x
 - ∘ '*' star; 's' square
 - 'v' triangle down; '^' triangle up
 - '<' triangle left; '>' triangle right
 - o 'p' pentagon; '8' octagon;
 - 'h' hexagon; 'd' thin_diamond
 - line styles:
 - ∘ '-' solid line
 - o '--' dashed line
 - o '-.' dash-dotted line
 - o ':' dotted lione

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Brief Review of Probability

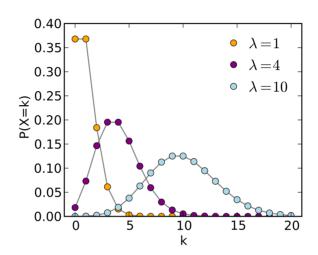
- Random variable (r.v.) X takes a value in ${\cal X}$ (set of possible values) at random.
- Associated with a probability distribution p(X) that describes the frequency of outcomes of the X.

Discrete random variables

- Probability mass function (pmf)
- p(X=x) is the probability of r.v. X taking value x
 - we will use simpler notation p(x)
- properties
 - $0 \le p(x) \le 1$
 - $lacksquare \sum_{x \in \mathcal{X}} p(x) = 1 \Rightarrow ext{"normalized to 1"}$

- 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 likelihood
 - $\int p(x)dx=1$, \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")
 - $lacksquare \operatorname{pdf:} p(x) = rac{1}{\sqrt{2\pi\sigma^2}} e^{-rac{1}{2\sigma^2}(x-\mu)^2}$

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: $p(x) = \sum_{y \in \mathcal{Y}} p(x,y)$
 - 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".

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

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

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

• 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,
 - lacksquare p(y|x)p(x) = p(x|y)p(y)
 - $p(y|x) = rac{p(x|y)p(y)}{p(x)}$
- Looking at denominator...
 - lacktriangledown marginalize: $p(x) = \int p(x,y) dy$

• Bayes' Rule

$$p(y|x) = \frac{p(x|y)p(y)}{\int p(x|y)p(y)dy}$$

- $p(y|x) = \frac{p(x|y)p(y)}{\int p(x|y)p(y)dy}$ 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