

# **INTRODUCTION TO DATA SCIENCE**

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**Lecture #5 – 09/15/2020**

**CMSC320**  
**Tuesdays & Thursdays**  
**5:00pm – 6:15pm**  
**(... or anytime on the Internet)**



**COMPUTER SCIENCE**  
UNIVERSITY OF MARYLAND

# ANNOUNCEMENTS

**Register on Piazza:** piazza.com/umd/fall2020/cmsc320

- 258 have registered already 
- ~-8 have not registered yet 

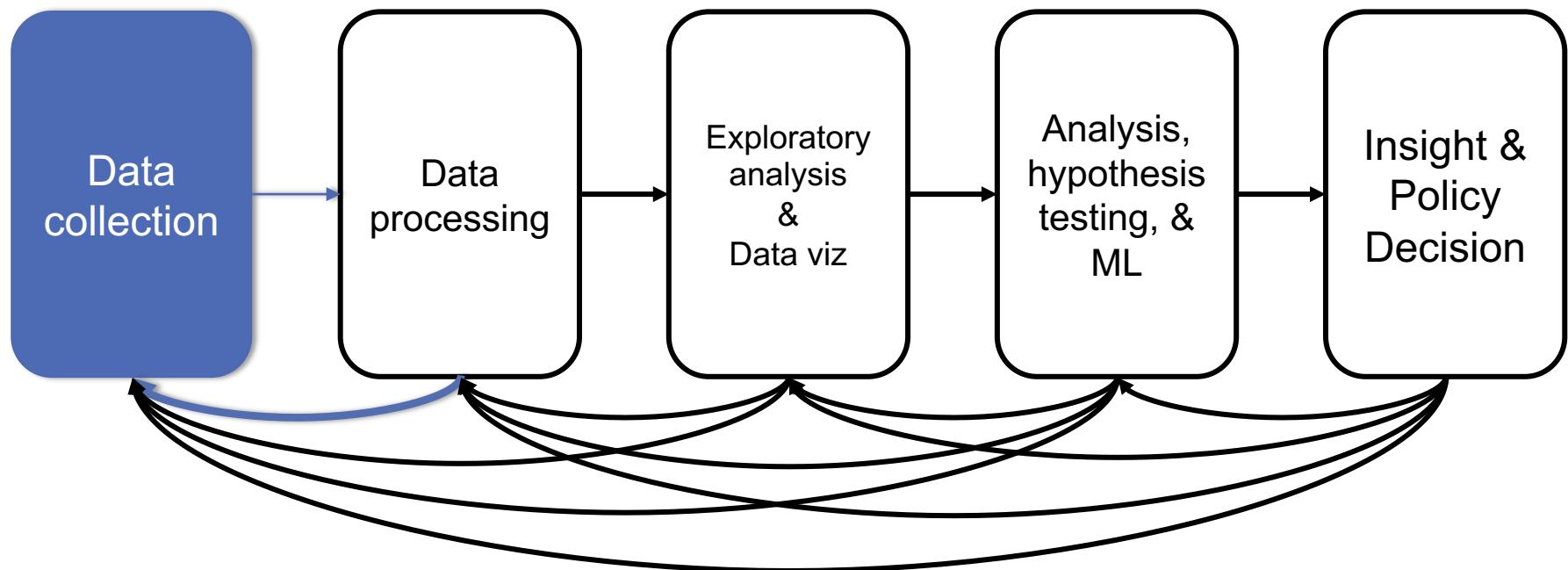
**If you were on Piazza, you'd know ...**

- **Project 1 is out now. (Worth 10% of grade, as are each of the four projects.)**
- Link is on course website @ cmsc320.github.io, also ELMS

**We've also linked some reading for the week!**

- Third **quiz** is due nexxt Tuesday at noon; on ELMS now.

# RECAP ...



# DOWNLOADING A BUNCH OF FILES

Import the modules

```
import re
import requests
from bs4 import BeautifulSoup
try:
    from urllib.parse import urlparse
except ImportError:
    from urlparse import urlparse
```

Get some HTML via HTTP

```
# HTTP GET request sent to the URL url
r = requests.get( url )

# Use BeautifulSoup to parse the GET response
root = BeautifulSoup( r.content )
lnks = root.find("div", id="schedule") \
    .find("table") \
    .find("tbody").findAll("a")
```

# DOWNLOADING A BUNCH OF FILES

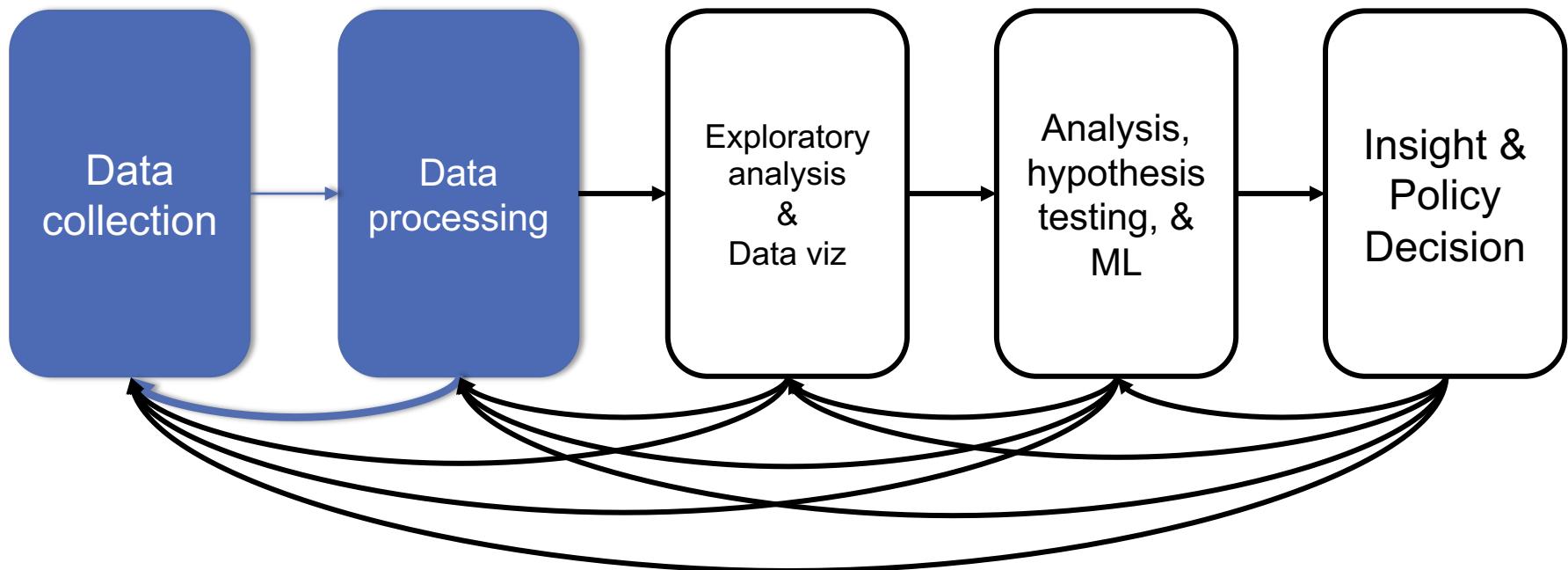
Parse exactly what you want

```
# Cycle through the href for each anchor, checking  
# to see if it's a PDF/PPTX link or not  
for lnk in lnks:  
    href = lnk['href']  
  
    # If it's a PDF/PPTX link, queue a download  
    if href.lower().endswith('.pdf', '.pptx'):
```

Get some more data?!

```
urld = urlparse.urljoin(url, href)  
rd = requests.get(urld, stream=True)  
  
# Write the downloaded PDF to a file  
outfile = path.join(outbase, href)  
with open(outfile, 'wb') as f:  
    f.write(rd.content)
```

# NEXT ...



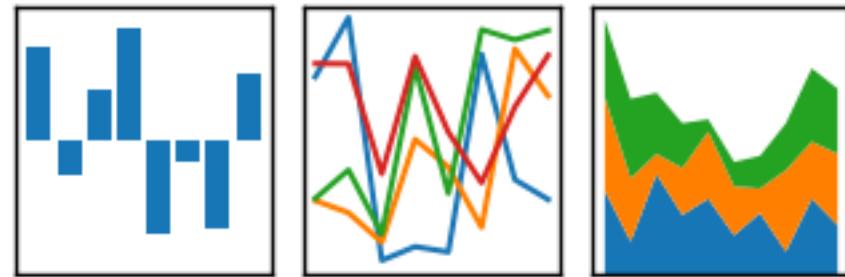


*NEXT UP:*

# NUMPY, SCIPY, AND DATAFRAMES

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$



# NEXT FEW CLASSES

## 1. NumPy: Python Library for Manipulating nD Arrays

Multidimensional Arrays, and a variety of operations including Linear Algebra

## 2. Pandas: Python Library for Manipulating Tabular Data

Series, Tables (also called **DataFrames**)

Many operations to manipulate and combine tables/series

## 3. Relational Databases

Tables/Relations, and SQL (similar to Pandas operations)

## 4. Apache Spark

Sets of objects or key-value pairs

MapReduce and SQL-like operations

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# **NUMERIC & SCIENTIFIC APPLICATIONS**

**Number of third-party packages available for numerical and scientific computing**

**These include:**

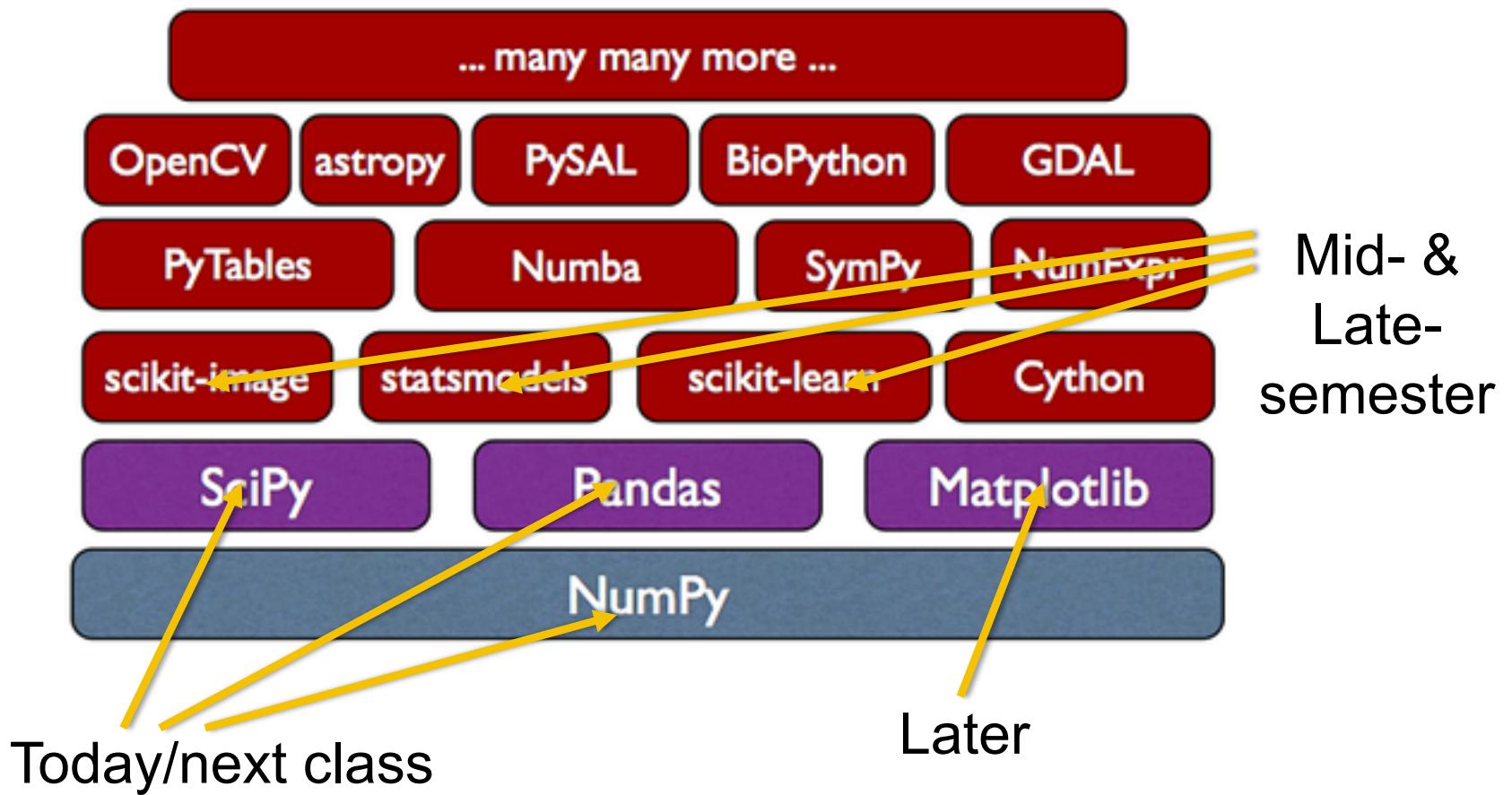
- NumPy/SciPy – numerical and scientific function libraries.
- numba – Python compiler that support JIT compilation.
- ALGLIB – numerical analysis library.
- pandas – high-performance data structures and data analysis tools.
- pyGSL – Python interface for GNU Scientific Library.
- ScientificPython – collection of scientific computing modules.

# **NUMPY AND FRIENDS**

**By far, the most commonly used packages are those in the NumPy stack. These packages include:**

- NumPy: similar functionality as Matlab
- SciPy: integrates many other packages like NumPy
- Matplotlib & Seaborn – plotting libraries
- iPython via Jupyter – interactive computing
- Pandas – data analysis library
- SymPy – symbolic computation library

# THE NUMPY STACK



# NUMPY

**Among other things, NumPy contains:**

- A powerful  $n$ -dimensional array object.
- Sophisticated (broadcasting/universal) functions.
- Tools for integrating C/C++ and Fortran code.
- Useful linear algebra, Fourier transform, and random number capabilities, etc.

**Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data.**



# NUMPY

**ndarray object: an  $n$ -dimensional array of homogeneous data types, with many operations being performed in compiled code for performance**

**Several important differences between NumPy arrays and the standard Python sequences:**

- NumPy arrays have a fixed size. Modifying the size means creating a new array.
- NumPy arrays must be of the same data type, but this can include Python objects – may not get performance benefits
- More efficient mathematical operations than built-in sequence types.

# NUMPY DATATYPES

Wider variety of data types than are built-in to the Python language by default.

Defined by the `numpy.dtype` class and include:

- `intc` (same as a C integer) and `intp` (used for indexing)
- `int8`, `int16`, `int32`, `int64`
- `uint8`, `uint16`, `uint32`, `uint64`
- `float16`, `float32`, `float64`
- `complex64`, `complex128`
- `bool_`, `int_`, `float_`, `complex_` are shorthand for defaults.

These can be used as functions to cast literals or sequence types, as well as arguments to NumPy functions that accept the `dtype` keyword argument.

# NUMPY DATATYPES

```
>>> import numpy as np
>>> x = np.float32(1.0)
>>> x
1.0
>>> y = np.int_(1,2,4)
>>> y
array([1, 2, 4])
>>> z = np.arange(3, dtype=np.uint8)
>>> z
array([0, 1, 2], dtype=uint8)
>>> z.dtype
dtype('uint8')
```

# NUMPY ARRAYS

**There are a couple of mechanisms for creating arrays in NumPy:**

- Conversion from other Python structures (e.g., lists, tuples)
  - Any sequence-like data can be mapped to a ndarray
- Built-in NumPy array creation (e.g., arange, ones, zeros, etc.)
  - Create arrays with all zeros, all ones, increasing numbers from 0 to 1 etc.
- Reading arrays from disk, either from standard or custom formats (e.g., reading in from a CSV file)

# NUMPY ARRAYS

In general, any numerical data that is stored in an array-like container can be converted to an `ndarray` through use of the `array()` function. The most obvious examples are sequence types like lists and tuples.

```
>>> x = np.array([2,3,1,0])  
  
>>> x = np.array([2, 3, 1, 0])  
  
>>> x = np.array([[1,2.0],[0,0],(1+1j,3.)])  
  
>>> x = np.array([[ 1.+0.j,  2.+0.j], [ 0.+0.j,  0.+0.j],  
[ 1.+1.j,  3.+0.j]])
```

# NUMPY ARRAYS

## Creating arrays from scratch in NumPy:

- zeros (shape) – creates an array filled with 0 values with the specified shape. The default dtype is float64.

```
>>> np.zeros((2, 3))
array([[ 0.,  0.,  0.], [ 0.,  0.,  0.]])
```

- ones (shape) – creates an array filled with 1 values.
- arange () – like Python's built-in range

```
>>> np.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> np.arange(2, 10, dtype=np.float)
array([ 2.,  3.,  4.,  5.,  6.,  7.,  8.,  9.])
>>> np.arange(2, 3, 0.2)
array([ 2.,  2.2,  2.4,  2.6,  2.8])
```

# NUMPY ARRAYS

`linspace()` – creates arrays with a specified number of elements, and spaced equally between the specified beginning and end values.

```
>>> np.linspace(1., 4., 6)
array([ 1. , 1.6, 2.2, 2.8, 3.4, 4. ])
```

`random.random(shape)` – creates arrays with random floats over the interval [0,1).

```
>>> np.random.random((2,3))
array([[ 0.75688597, 0.41759916, 0.35007419],
       [ 0.77164187, 0.05869089, 0.98792864]])
```

# NUMPY ARRAYS

Printing an array can be done with the `print`

- statement (Python 2)
- function (Python 3)

```
>>> import numpy as np
>>> a = np.arange(3)
>>> print(a)
[0 1 2]
>>> a
array([0, 1, 2])
>>> b = np.arange(9).reshape(3,3)
>>> print(b)
[[0 1 2]
 [3 4 5]
 [6 7 8]]
>>> c =
np.arange(8).reshape(2,2,2)
>>> print(c)
[[[0 1]
 [2 3]]

 [[4 5]
 [6 7]]]
```

# INDEXING

Single-dimension indexing is accomplished as usual.

```
>>> x = np.arange(10)
>>> x[2]
2
>>> x[-2]
8
```

Multi-dimensional arrays support multi-dimensional indexing.

```
>>> x.shape = (2,5) # now x is 2-dimensional
>>> x[1,3]
8
>>> x[1,-1]
9
```

# INDEXING

Using fewer dimensions to index will result in a subarray:

```
>>> x = np.arange(10)
>>> x.shape = (2, 5)
>>> x[0]
array([0, 1, 2, 3, 4])
```

This means that `x[i, j] == x[i][j]` but the second method is less efficient.

# INDEXING

Slicing is possible just as it is for typical Python sequences:

```
>>> x = np.arange(10)
>>> x[2:5]
array([2, 3, 4])
>>> x[:-7]
array([0, 1, 2])
>>> x[1:7:2]
array([1, 3, 5])
>>> y = np.arange(35).reshape(5,7)
>>> y[1:5:2, ::3]
array([[ 7, 10, 13], [21, 24, 27]])
```

# ARRAY OPERATIONS

Basic operations apply element-wise. The result is a new array with the resultant elements.

```
>>> a = np.arange(5)
>>> b = np.arange(5)
>>> a+b
array([0, 2, 4, 6, 8])
>>> a-b
array([0, 0, 0, 0, 0])
>>> a**2
array([ 0,  1,  4,  9, 16])
>>> a>3
array([False, False, False, False, True], dtype=bool)
>>> 10*np.sin(a)
array([ 0.,  8.41470985,  9.09297427,  1.41120008, -7.56802495])
>>> a*b
array([ 0,  1,  4,  9, 16])
```

# ARRAY OPERATIONS

Since multiplication is done element-wise, you need to specifically perform a dot product to perform matrix multiplication.

```
>>> a = np.zeros(4).reshape(2,2)
>>> a
array([[ 0.,  0.],
       [ 0.,  0.]])
>>> a[0,0] = 1
>>> a[1,1] = 1
>>> b = np.arange(4).reshape(2,2)
>>> b
array([[0, 1],
       [2, 3]])
>>> a*b
array([[ 0.,  0.],
       [ 0.,  3.]])
>>> np.dot(a,b)
array([[ 0.,  1.],
       [ 2.,  3.]])
```

# ARRAY OPERATIONS

**There are also some built-in methods of ndarray objects.**

**Universal functions which may also be applied include exp, sqrt, add, sin, cos, etc.**

```
>>> a = np.random.random((2, 3))
>>> a
array([[ 0.68166391,  0.98943098,
        0.69361582],
       [ 0.78888081,  0.62197125,
        0.40517936]])
>>> a.sum()
4.1807421388722164
>>> a.min()
0.4051793610379143
>>> a.max(axis=0)
array([ 0.78888081,  0.98943098,
        0.69361582])
>>> a.min(axis=1)
array([ 0.68166391,  0.40517936])
```

# ARRAY OPERATIONS

An array shape can be manipulated by a number of methods.

`resize(size)` will modify an array in place.

`reshape(size)` will return a copy of the array with a new shape.

```
>>> a =  
np.floor(10*np.random.random((3,4)))  
>>> print(a)  
[[ 9.  8.  7.  9.]  
 [ 7.  5.  9.  7.]  
 [ 8.  2.  7.  5.]]  
>>> a.shape  
(3, 4)  
>>> a.ravel()  
array([ 9.,  8.,  7.,  9.,  7.,  5.,  9.,  
       7.,  8.,  2.,  7.,  5.])  
>>> a.shape = (6,2)  
>>> print(a)  
[[ 9.  8.]  
 [ 7.  9.]  
 [ 7.  5.]  
 [ 9.  7.]  
 [ 8.  2.]  
 [ 7.  5.]]  
>>> a.transpose()  
array([[ 9.,  7.,  7.,  9.,  8.,  7.],  
       [ 8.,  9.,  5.,  7.,  2.,  5.]])
```

# LINEAR ALGEBRA

One of the most common reasons for using the NumPy package is its linear algebra module.

It's like Matlab, but free!

```
>>> from numpy import *
>>> from numpy.linalg import *
>>> a = array([[1.0, 2.0],
              [3.0, 4.0]])
>>> print(a)
[[ 1.  2.]
 [ 3.  4.]]
>>> a.transpose()
array([[ 1.,  3.],
       [ 2.,  4.]])
>>> inv(a) # inverse
array([[-2.,  1.],
       [ 1.5, -0.5]])
```

# LINEAR ALGEBRA

```
>>> u = eye(2) # unit 2x2 matrix; "eye" represents "I"
>>> u
array([[ 1.,  0.],
       [ 0.,  1.]])
>>> j = array([[0.0, -1.0], [1.0,  0.0]])
>>> dot(j, j) # matrix product
array([[-1.,  0.],
       [ 0., -1.]])
>>> trace(u) # trace (sum of elements on diagonal)
2.0
>>> y = array([[5.], [7.]])
>>> solve(a, y) # solve linear matrix equation
array([[-3.],
       [ 4.]])
>>> eig(j) # get eigenvalues/eigenvectors of matrix
(array([ 0.+1.j,  0.-1.j]),
 array([[ 0.70710678+0.j,  0.70710678+0.j],
       [ 0.00000000-0.70710678j,
       0.00000000+0.70710678j]]))
```

# SCIPY?



**In its own words:**

SciPy is a collection of mathematical algorithms and convenience functions **built on the NumPy extension** of Python. It adds significant power to the interactive Python session by providing the user with high-level commands and classes for manipulating and visualizing data.

**Basically, SciPy contains various tools and functions for solving common problems in scientific computing.**

# SCIPY

SciPy gives you access to a ton of specialized mathematical functionality.

- **Just know it exists. We won't use it much in this class.**

**Some functionality:**

- Special mathematical functions (scipy.special) -- elliptic, bessel, etc.
- Integration (scipy.integrate)
- Optimization (scipy.optimize)
- Interpolation (scipy.interpolate)
- Fourier Transforms (scipy.fftpack)
- Signal Processing (scipy.signal)
- Linear Algebra (scipy.linalg)
- Compressed Sparse Graph Routines (scipy.sparse.csgraph)
- Spatial data structures and algorithms (scipy.spatial)
- Statistics (scipy.stats)
- Multidimensional image processing (scipy.ndimage)
- Data IO (scipy.io) – overlaps with pandas, covers some other formats

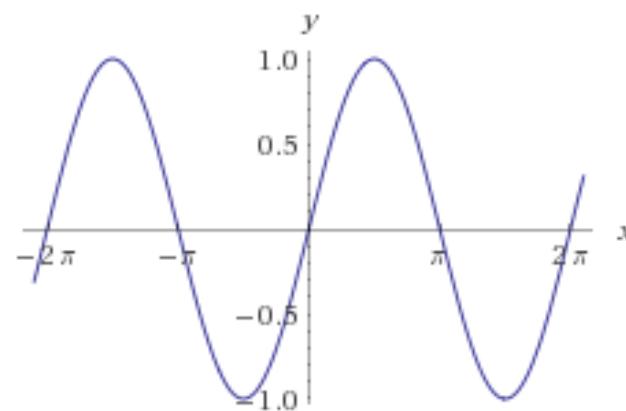
# ONE SCIPY EXAMPLE

We can't possibly tour all of the SciPy library and, even if we did, it might be a little boring.

- Often, you'll be able to find higher-level modules that will work around your need to directly call low-level SciPy functions

Say you want to compute an integral:

$$\int_a^b \sin x \, dx$$



# SCIPY.INTEGRATE

We have a function object – `np.sin` defines the sin function for us.

We can compute the definite integral from  $x = 0$  to  $x = \pi$  using the `quad` function.

```
>>> res = scipy.integrate.quad(np.sin, 0, np.pi)
>>> print(res)
(2.0, 2.220446049250313e-14) # 2 with a very small error
margin!
>>> res = scipy.integrate.quad(np.sin, -np.inf, +np.inf)
>>> print(res)
(0.0, 0.0) # Integral does not converge
```

# SCIPY.INTEGRATE

Let's say that we don't have a function object, we only have some (x,y) samples that "define" our function.

We can estimate the integral using the trapezoidal rule.

```
>>> sample_x = np.linspace(0, np.pi, 1000)
>>> sample_y = np.sin(sample_x) # Creating 1,000 samples
>>> result = scipy.integrate.trapz(sample_y, sample_x)
>>> print(result)
1.99999835177

>>> sample_x = np.linspace(0, np.pi, 1000000)
>>> sample_y = np.sin(sample_x) # Creating 1,000,000
samples
>>> result = scipy.integrate.trapz(sample_y, sample_x)
>>> print(result)
2.0
```

# **WRAP UP: FIRST PART**

**Shift thinking from imperative coding to operations on datasets**

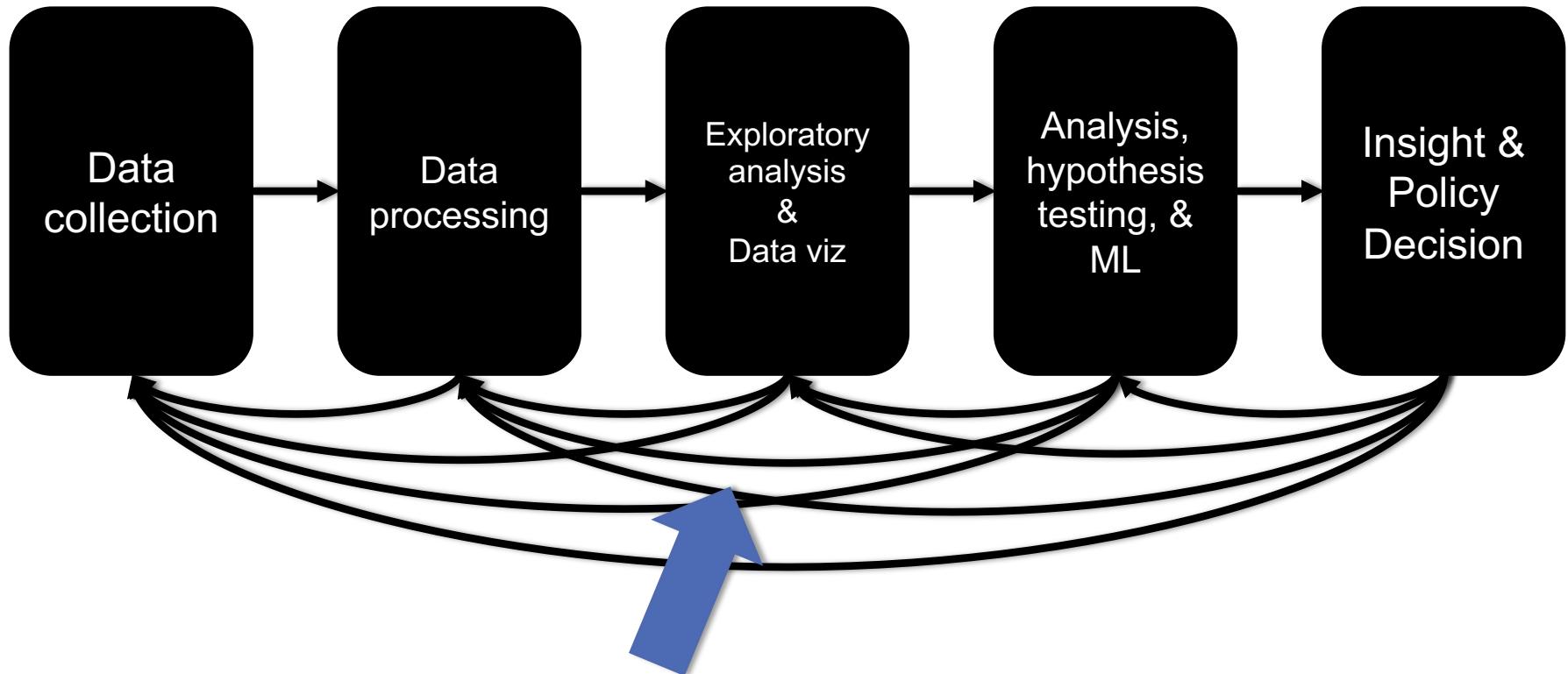
**Numpy: A low-level abstraction that gives us really fast multi-dimensional arrays**

**Next class:**

**Pandas: Higher-level tabular abstraction and operations to manipulate and combine tables**

**Reading Homework focuses on Pandas and SQL**

# REMAINDER OF TODAY'S LECTURE



Quick best practices  
for managing this monstrosity.

# REPRODUCIBILITY

**Extremely important aspect of data analysis**

- “Starting from the same raw data, can we reproduce your analysis and obtain the same results?”

**Using libraries helps:**

- Since you don’t reimplement everything, reduce programmer error
- Large user bases serve as “watchdog” for quality and correctness

**Standard practices help:**

- Version control: git, git, git, ..., git, svn, cvs, hg, Dropbox
- Unit testing: unittest (Python), RUnit (R), testthat
- Share and publish: github, gitlab

# REPRODUCIBILITY

## Open data:

“**Open data** is the idea that some data should be freely available to everyone to use and republish as they wish, without restrictions from copyright, patents or other mechanisms of control”

## Open Data movement website

- <http://www.opendatafoundation.org/>



# PRACTICAL TIPS

Many tasks can be organized in modular manner:

- Data acquisition:
  - Get data, put it in usable format (many ‘join’ operations), clean it up
- Algorithm/tool development:
  - If new analysis tools are required
- Computational analysis:
  - Use tools to analyze data
- Communication of results:
  - Prepare summaries of experimental results, plots, publication, upload processed data to repositories

Usually a single language or tool does not handle all of these equally well – **choose the best tool for the job!**

# PRACTICAL TIPS

**Modularity requires organization and careful thought**

**In Data Science, we wear two hats:**

- Algorithm/tool developer
- **Experimentalist**: we don't get trained to think this way enough!

**It helps to consciously separate these two jobs**

# **THINK LIKE AN EXPERIMENTALIST**

**Plan your experiment**

**Gather your raw data**

**Gather your tools**

**Execute experiment**

**Analyze**

**Communicate**



# THINK LIKE AN EXPERIMENTALIST

Let this guide your organization. One potential structure for organizing a project:

```
project/
|   data/
|   |   processing_scripts
|   |   raw/
|   |   proc/
|   tools/
|   |   src/
|   |   bin/
|   exps
|   |   pipeline_scripts
|   |   results/
|   |   analysis_scripts
|   |   figures/
```

# THINK LIKE AN EXPERIMENTALIST

**Keep a lab notebook!**

**Literate programming tools are making this easier for computational projects:**

- [http://en.wikipedia.org/wiki/Literate\\_programming](http://en.wikipedia.org/wiki/Literate_programming) (Lec #2!)
- <https://ipython.org/>
- <http://rmarkdown.rstudio.com/>
- <http://jupyter.org/>

# THINK LIKE AN EXPERIMENTALIST

## Separate experiment from analysis from communication

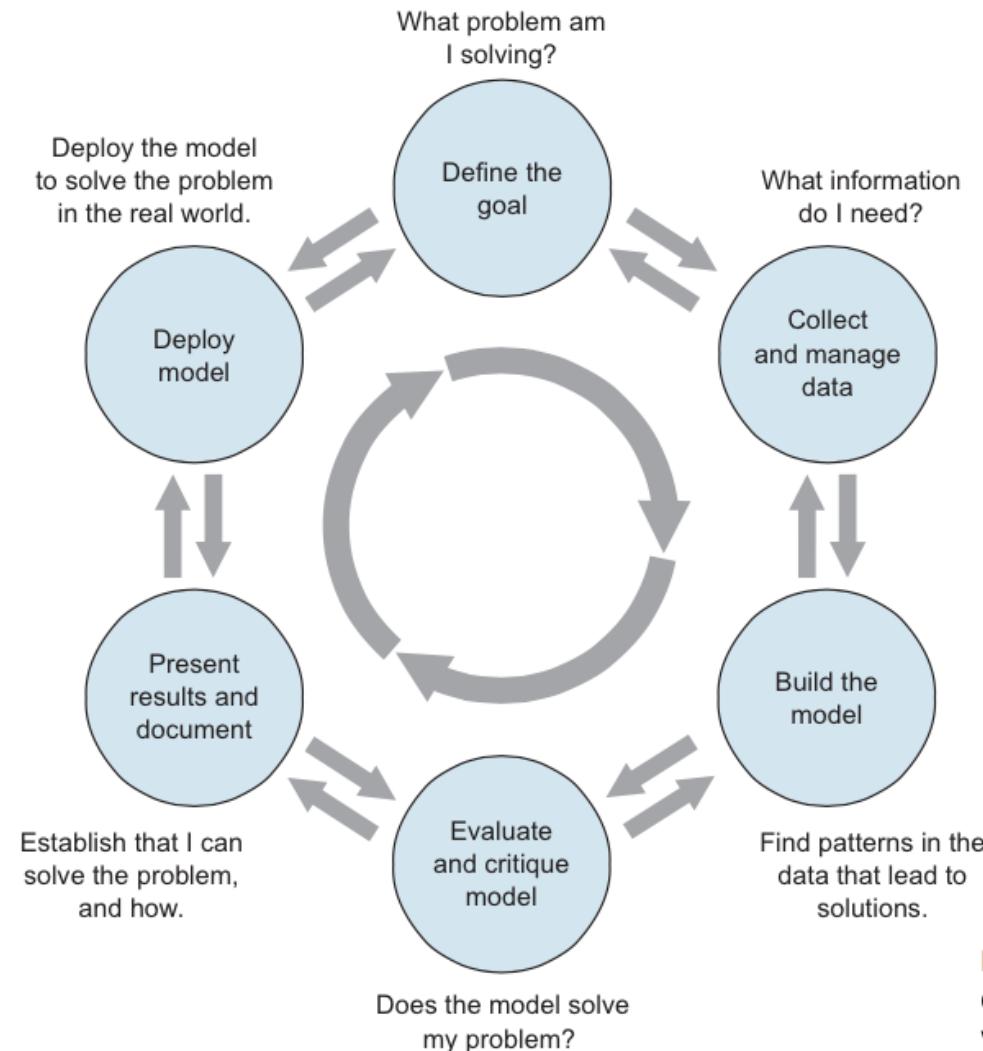
- Store results of computations, write separate scripts to analyze results and make plots/tables

## Aim for reproducibility

- There are serious consequences for not being careful
  - Publication retraction
  - Worse:  
[http://videolectures.net/cancerbioinformatics2010\\_baggerly\\_irrh/](http://videolectures.net/cancerbioinformatics2010_baggerly_irrh/)
- Lots of tools available to help, use them! Be proactive: learn about them on your own!

# **BIAS, ETHICS, & RESPONSIBILITY**

# DATA SCIENCE LIFECYCLE: AN ALTERNATE VIEW



**Figure 1.1** The lifecycle of a data science project: loops within loops

# EXAMPLES OF BIAS

## Genetic testing

- Genetic tests for heart disorder and race-biased risk (NYTimes)
- Race-bias in ancestry reports

## Search results / feed optimization

- Google
- Facebook

# **COMBATING BIAS**

**Fairness through blindness:**

- Don't let an algorithm look at **protected attributes**

**Examples currently in use ??????????**

- Race
- Gender
- Sexuality
- Disability
- Religion

**Problems with this approach ??????????**

# COMBATING BIAS

## Demographic parity:

- A decision must be independent of the protected attribute
- E.g., a loan application's acceptance rate is independent of an applicant's race (but can be dependent on non-protected features like salary)

**Formally: binary decision variable C, protected attribute A**

- $P\{ C = 1 | A = 0 \} = P\{ C = 1 | A = 1 \}$

**Membership in a protected class should have no correlation with the final decision.**

- Problems ????????

# COMBATING BIAS

## What if the decision isn't the thing that matters?

“Consider, for example, a luxury hotel chain that renders a promotion to a subset of wealthy whites (who are likely to visit the hotel) and a subset of less affluent blacks (who are unlikely to visit the hotel). The situation is obviously quite icky, but demographic parity is completely fine with it so long as the same fraction of people in each group see the promotion.”

**Demographic parity allows classifiers that select qualified candidates in the “majority” demographic and unqualified candidate in the “minority” demographic, within a protected attribute, so long as the expected percentages work out.**

More: <http://blog.mrtz.org/2016/09/06/approaching-fairness.html>

# FATML

**This stuff is really tricky (and really important).**

- It's also not solved, even remotely, yet!
- CMSC498/499 ❤

**New community: Fairness, Accountability, and Transparency in Machine Learning (aka FATML)**

“... policymakers, regulators, and advocates have expressed fears about the potentially discriminatory impact of machine learning, with many calling for further technical research into the dangers of inadvertently encoding bias into automated decisions.”



**Fairness, Accountability,  
and Transparency  
in Machine Learning**

# **F IS FOR FAIRNESS**

**In large data sets, there is always proportionally less data available about minorities.**

**Statistical patterns that hold for the majority may be invalid for a given minority group.**

**Fairness can be viewed as a measure of diversity in the combinatorial space of sensitive attributes, as opposed to the geometric space of features.**

# A IS FOR ACCOUNTABILITY

**Accountability of a mechanism implies an obligation to report, explain, or justify algorithmic decision-making as well as mitigate any negative social impacts or potential harms.**

- Current accountability tools were developed to oversee human decision makers
- They often fail when applied to algorithms and mechanisms instead

**Example, no established methods exist to judge the intent of a piece of software. Because automated decision systems can return potentially incorrect, unjustified or unfair results, additional approaches are needed to make such systems accountable and governable.**

# T IS FOR TRANSPARENCY

**Automated ML-based algorithms make many important decisions in life.**

- Decision-making process is opaque, hard to audit

**A transparent mechanism should be:**

- understandable;
- more meaningful;
- more accessible; and
- more measurable.

# **DATA COLLECTION**

**What data should (not) be collected**

**Who owns the data**

**Whose data can (not) be shared**

**What technology for collecting, storing, managing data**

**Whose data can (not) be traded**

**What data can (not) be merged**

**What to do with prejudicial data**

# DATA MODELING

## Data is biased (known/unknown)

- Invalid assumptions
- Confirmation bias

## Publication bias

- WSDM 2017: <https://arxiv.org/abs/1702.00502>

## Badly handling missing values

# DEPLOYMENT

**Spurious correlation / over-generalization**

**Using “black-box” methods that cannot be explained**

**Using heuristics that are not well understood**

**Releasing untested code**

**Extrapolating**

**Not measuring lifecycle performance (concept drift in ML)**

**We will go over ways to counter  
this in the ML/stats/hypothesis  
testing portion of the course**

# **GUIDING PRINCIPLES**

**Start with clear user need and public benefit**

**Use data and tools which have minimum intrusion necessary**

**Create robust data science models**

**Be alert to public perceptions**

**Be as open and accountable as possible**

**Keep data secure**



# SOME REFERENCES

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*NEXT CLASS:*

# **PANDAS, TIDY DATA & (MAYBE) START ON RELATIONAL MODEL OF DATA**

