INTRODUCTION TO DATA SCIENCE

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Lecture #4 – 09/09/2021
Lecture #5 – 09/14/2021

CMSC320
Tuesdays & Thursdays
5:00pm – 6:15pm

https://cmsc320.github.io/

COMPUTER SCIENCE
UNIVERSITY OF MARYLAND

ANNOUNCEMENTS

Register on Piazza: piazza.com/umd/fall2021/cmsc320

- XXX have registered already ♡
- Very few have not registered yet ♡

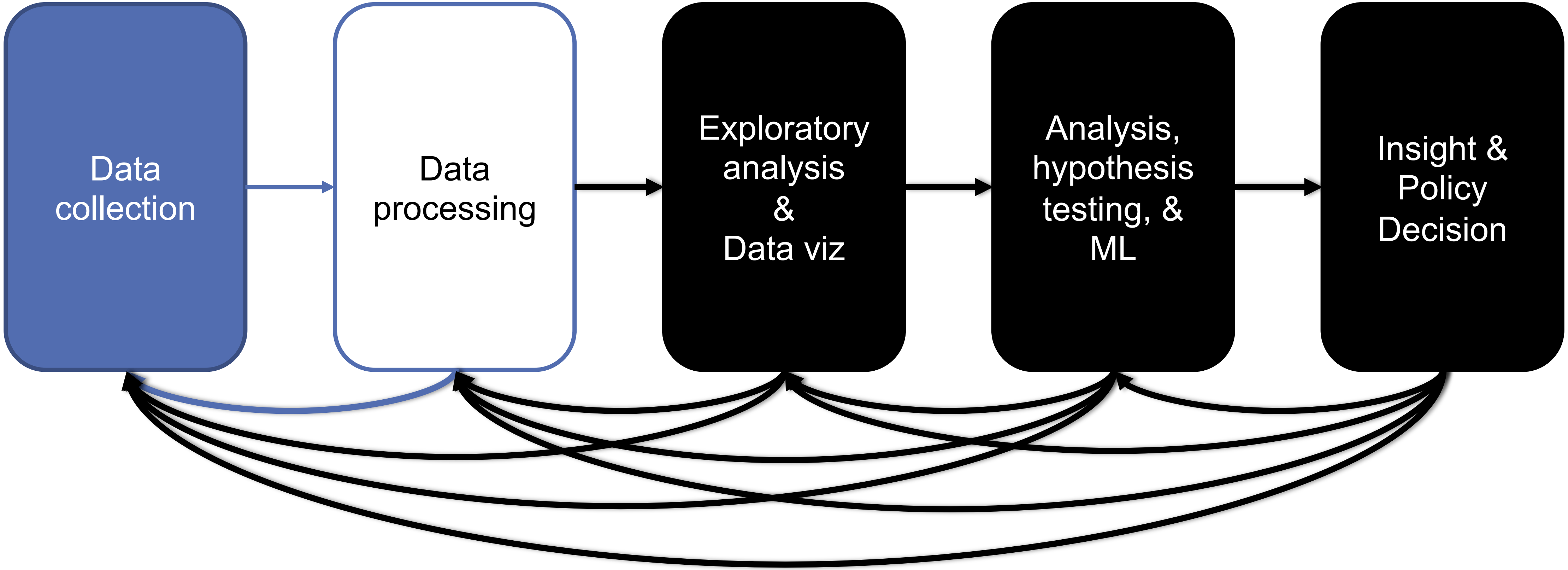
If you were on Piazza, you'd know …

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

We've also linked some reading for the week!

- Quizzes are generally due on Tuesdays at noon; on ELMS now.

THE DATA LIFECYCLE


Data collection
Data processing
Exploratory analysis & Data viz
Analysis, hypothesis testing, & ML
Insight & Policy Decision

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.

Many, many thanks to: FSU CIS4930

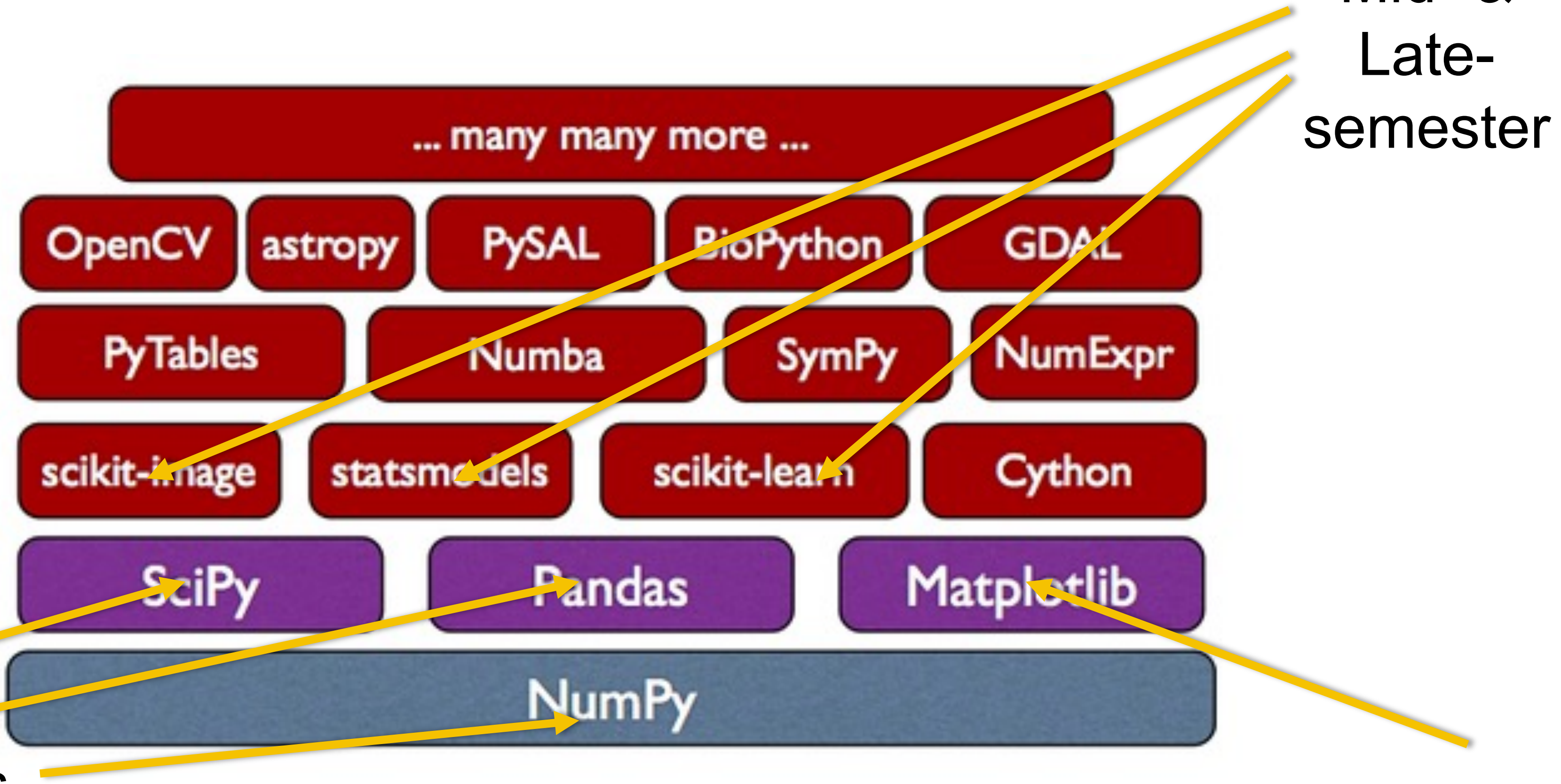
NUMPY AND FRIENDS

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

[FSU]

THE NUMPY STACK



Mid- &
Late-
semester

Today/next class

Later

Image from Continuum Analytics

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.

[FSU]

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.

[FSU]

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.

[FSU]

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)

[FSU]

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.]])
```

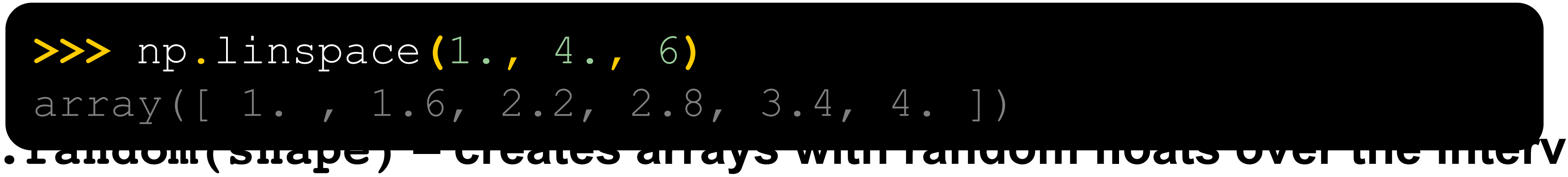
- `ones(shape)` – creates an array filled with 1 values.
- `arange()` – like Python’s built-in `range`

```
>>> 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])
```

[FSU]

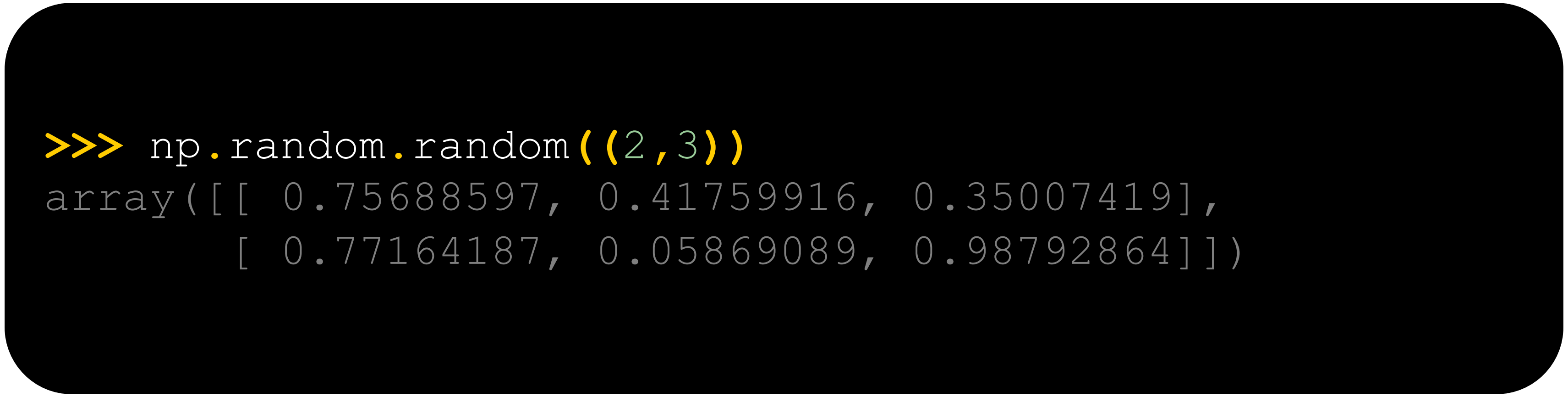
NUMPY ARRAYS

`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]])
```

[FSU]

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

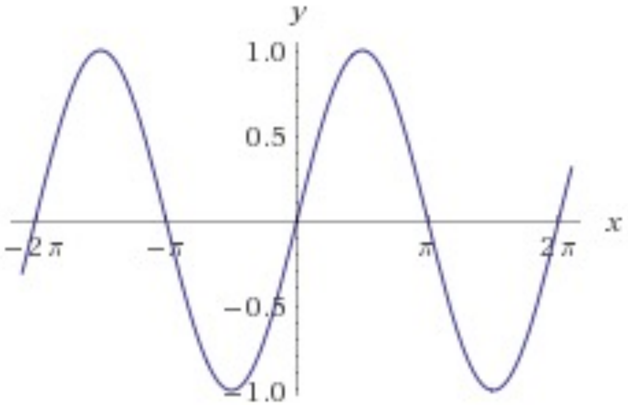
ONE SCIPY EXAMPLE

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