HINF 5502: Third-party Python software and distributions

This is a demonstration notebook of some of the packages discussed in the Week 11 lecture. I have some commentary inside, but note that I may have more commentary in my recorded lecture. If you've installed the Anaconda Python (http://continuum.io) distribution, you should have all of the tools you need.

First, let's import the packages, which I'll do in one step. We're using the convention of `import ... as ...`, which will let us use functions and objects in the modules using abbreviations. You can use any abbreviation you want, but the abbreviations below have become the conventional ways to refer to these major packages. The last command is actually one for the notebook system, and tells it to take any graphics generated by Matplotlib (http://www.matplotlib.org) (or Seaborn) and paste them into the notebook "inline" by default.

```
In [1]: import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        import seaborn as sns
        %matplotlib inline
```

NumPy (http://www.numpy.org/) implements fast and efficient arrays, which are like Python lists, but are generally restricted to one data type for all of the elements. This may seem like a step backwards, but by constraining arrays to one data type, a lot of things are made faster. The NumPy package also brings a host of mathematical and other functions to work on arrays, many more than what come with Python itself.

When we think of arrays in a mathematical sense, we usually think of two-dimensional arrays and linear algebra. While NumPy does not just work with 2D arrays (they can be 1D, 3D, or any dimension), we can do a lot of linear algebra operations, which typically involve 2D numerical arrays. For example, we can create the 2D array

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

using the `np.array()` function. Note that it looks mostly like a list of lists:

```
In [2]: my_matrix = np.array([[1, 2], [3, 4]])
        my_matrix
```

```
Out[2]: array([[1, 2],
               [3, 4]])
```

As you might expect, we can do all kinds of linear algebra "things" to this array, such as finding the inverse:

In [3]:
```
my_matrix_inv = np.linalg.inv(my_matrix)
my_matrix_inv
```

Out[3]:
```
array([[-2. ,  1. ],
       [ 1.5, -0.5]])
```

If we multiplied the two matrices together using standard matrix multiplication, we'd get the identity matrix. (If you're not familiar with linear algebra and don't know what this means, don't worry!)

More interesting is using the arrays to solve systems of linear equations. If you've taken linear algebra and done things like Gaussian elimination to solve such systems, you can do the same thing with NumPy. Here is a system of four equations and four unknowns:

$$\begin{aligned} 2w - x + 5y + z &= -3 \\ 3w + 2x + 2y - 6z &= -32 \\ w + 3x + 3y - z &= -47 \\ 5w - 2x - 3y + 3z &= 49 \end{aligned}$$

Solving this is actually pretty easy. We can take the coefficients on each side of the equations, and make them into arrays, then plug them into `np.linalg.solve()` :

In [4]:
```
leftside = np.array([[2, -1, 5, 1], [3, 2, 2, -6], [1, 3, 3, -1], [5, -2, -3, 3]]
rightside = np.array([-3, -32, -47, 49])
solution = np.linalg.solve(leftside, rightside)
solution
```

Out[4]:
```
array([  2., -12.,  -4.,   1.])
```

```
Thus, *w* = 2, *x* = -12, *y* = -4, and *z* = 1. If you plug those numbers
into the equations, all of them will work.
```

### Random number generation and plotting

```
Here's something a little more interesting. We'll make a 1D array composed of
10,000 random normally-distributed numbers, with a mean of 100, and a standard
deviation of 20. The base Python distribution, using the `random` library, can
generate these numbers, but NumPy has its own functions to do this. The first
command sets the *seed* for the random number generator, so that I can
generate the same list of random numbers each time I run this (and you can,
too). The third command shows us the first ten numbers generated.
```

In [5]:
```
np.random.seed(5502) # I can use any number here, and just chose the course numbe
my_sample = np.random.normal(100, 20, 10000)
my_sample[0:10]
```

Out[5]:
```
array([ 94.33524784, 108.02934025,  97.35417356,  99.25560324,
       100.65609013, 122.10688732,  92.2056135 , 101.84476819,
       110.17498942,  88.46646567])
```

We can use Matplotlib to generate a histogram of the 10,000 numbers. The different commands set different options and aspects of the plot.

In [ ]:
```
plt.hist(my_sample, 50)
plt.title("Histogram of random normal variates")
plt.xlabel("Value")
plt.ylabel("Frequency")
plt.show()
```

This looks pretty much like a normal distribution. It's not perfect, but it only has 10,000 numbers in it. As we add more numbers, it would smooth out further, but this is pretty good already.

```
### Speed and efficiency

So far, aside from the functions that do linear algebra, it's hard to see what
the advantage of NumPy is over just using built-in Python lists. We can
illustrate this with an example, though. Let's take our NumPy array of the
random numbers, then calculate their reciprocals (*i.e.*, if a number is *x*,
then calculate 1/*x*). First, let's convert the NumPy array into an ordinary
list:
```

In [6]:
```
my_list = list(my_sample)
```

Now, calculate the reciprocals and put them in a new list. I'm using a list comprehension to do this, but it could just as easily be set up as a `for` loop. Then we'll take a peek at the first ten reciprocals.

In [7]:
```
my_reciprocals1 = [1/x for x in my_list]
my_reciprocals1[0:10]
```

Out[7]:
```
[0.010600491575711305,
 0.009256744488739277,
 0.010271773293757221,
 0.010074997958411944,
 0.00993481863543973,
 0.008189546240683436,
 0.010845326678065622,
 0.009818864706872389,
 0.00907647012472204,
 0.011303718221963917]
```

```
Nothing very controversial here. Now, let's create a NumPy array of the
reciprocals. Below is the command to do it. Note that it's not a `for` loop,
nor is it a comprehension. In fact, it looks like a very simple calculation.
This is one of the NumPy advantages: arrays are *vectorized*, meaning that if
we apply a mathematical function to an array, it's understood that the
function should be applied to every element in the array automatically! Here,
it's understood that this new array is to be composed of the reciprocals of
the original array.

Because `my_reciprocals2` is a NumPy array object, the output is formatted a
little differently when printed. That's why we see the first ten reciprocals
in two rows this time, and with fewer decimal places.
```

In [8]:
```
my_reciprocals2 = 1 / my_sample
my_reciprocals2[0:10]
```

Out[8]:
```
array([0.01060049, 0.00925674, 0.01027177, 0.010075  , 0.00993482,
       0.00818955, 0.01084533, 0.00981886, 0.00907647, 0.01130372])
```

Here is where it gets more interesting. The notebook system has a mechanism to find the running times of commands. For the first command, we are timing the base Python list version of the reciprocal calculations. In the second command, we're timing the NumPy version.

In [12]:
```
%timeit my_reciprocals1 = [1/x for x in my_list]
```

```
4.69 ms ± 875 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

In [13]:
```
%timeit my_reciprocals2 = 1 / my_sample
```

```
14.1 µs ± 766 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

The commands were run 100 and 10,000 times, respectively, and the best timings were reported. It took about 1.7 milliseconds for the reciprocals to be calculated using the Python lists on my work iMac, and 8.4 *micro*seconds for the NumPy calculations to finish. Basically, the NumPy version ran over 200 times faster! Again, this is due to the way in which the NumPy arrays are implemented, as well as how the vectorization works.

From our standpoint, this isn't very much time in either instance, but imagine if you were calculating millions of such numbers. The time savings would add up quickly!

Pandas and data manipulation

For the last part of this demonstration, we'll use the Pandas (http://pandas.pydata.org/) package to do some data manipulation. Pandas is actually written with NumPy as its basis. The `DataFrame` object that Pandas defines is actually a special form of a NumPy array. The easiest way to think about this is is NumPy arrays are extremely efficient versions of Python lists, Pandas data frames are extremely efficient versions of Python dictionaries. That is, we can have keys of an arbitrary nature to refer to different values. Another way of thinking about this is that Pandas data frames are much like data frames in R, if you have worked with that statistical software package: we can have multiple lists put together in one structure. Each list is of a particular data type (strings, numbers, dates, *etc.*), but different lists can have different types. This is a natural way of thinking about rectangular, tabular data, such as is used in statistical software. It's also much like some of the data files we've practiced reading and calculating with in this course.

Let's read in two files with data. One is a file consisting of seven synthetic (fake) pediatric patients staying at a hospital, and the second is real data on 2013-2014 participants in the NHANES (http://www.cdc.gov/nchs/nhanes.htm) (National Health and Nutrition Examination Survey) study, a long-term study that has gone on for several decades in the United States. The pediatric data is in a tab-delimited format, and the NHANES data is in a comma-delimited format. We've practiced reading in tab-delimited data in this course, and you can probably figure out how to read in comma-delimited data as well. Pandas has functions to not only read this data in, but automatically turn it into data frame objects. Much easier than writing all the code yourself!

If you have the two data files in the same folder as this notebook, you can run the code below without changes.

In [14]:
```
patients = pd.read_table("patients.txt")
nhanes = pd.read_csv("nhanes.csv")
```

```
We'll take a look at the pediatric patient data first. The notebook interface
automatically takes the data and formats it as an easy-to-read table, which is
a nice bonus:
```

In [15]:
```
patients
```

Out[15]:

	patientid	lastname	firstname	birthdate	sex	admit	discharge	los	physician	dx1
0	55421	Blaine	Richard	1/5/12	M	11/30/15	12/30/15	31	Anderson	300.01
1	55426	Lazlo	Ilsa	7/6/10	F	11/10/15	11/21/15	12	Anderson	518.81
2	55427	Lazlo	Victor	5/13/07	M	11/2/15	11/3/15	2	Jones	493.22
3	55983	Renault	Louis	3/25/04	M	11/1/15	11/2/15	2	Jones	518.81
4	55678	Strasser	Heinrich	4/30/07	M	11/4/15	11/5/15	2	Gonzalez	493.02
5	55900	Ugarte	Peter	1/5/13	M	11/8/15	11/19/15	12	Gonzalez	518.81
6	55801	Ferrari	Sidney	4/5/08	F	11/10/15	11/21/15	12	Gonzalez	493.02

Here we have patient ID number, last name, first name, birthdate, sex, admit and discharge dates from the hospital, length of stay (LOS), the attending physician's name, and the patient's primary diagnosis as an ICD-9 code. ICD-9 is an older coding system for diseases and conditions, and was used in the US from 1988 to 2015. Let's suppose we wanted to find the current ages of the patients, derived from the birthdates. When first read in, anything that is not strictly a number is interpreted as a string by Pandas. As such, the dates in the data are just considered strings. However, Pandas (and NumPy) have a special date data type, which can make it easy to do date arithmetic. It's not hard to convert the string birthdates into objects Pandas actually understands as calendar dates.

The following command takes all the data in the `birthdate` column and turns it into Datetime objects.

In [16]:
```
pd.to_datetime(patients["birthdate"])
```

Out[16]:
```
0   2012-01-05
1   2010-07-06
2   2007-05-13
3   2004-03-25
4   2007-04-30
5   2013-01-05
6   2008-04-05
Name: birthdate, dtype: datetime64[ns]
```

We can then make a command that takes these objects and replaces the original strings with the new dates. Note how easy it is to specify that we want to replace all the data. No loops are required! We'll then look at the data a second time.

In [17]:
```
patients["birthdate"] = pd.to_datetime(patients["birthdate"])
patients
```

Out[17]:

	patientid	lastname	firstname	birthdate	sex	admit	discharge	los	physician	dx1
0	55421	Blaine	Richard	2012-01-05	M	11/30/15	12/30/15	31	Anderson	300.01
1	55426	Lazlo	Ilsa	2010-07-06	F	11/10/15	11/21/15	12	Anderson	518.81
2	55427	Lazlo	Victor	2007-05-13	M	11/2/15	11/3/15	2	Jones	493.22
3	55983	Renault	Louis	2004-03-25	M	11/1/15	11/2/15	2	Jones	518.81
4	55678	Strasser	Heinrich	2007-04-30	M	11/4/15	11/5/15	2	Gonzalez	493.02
5	55900	Ugarte	Peter	2013-01-05	M	11/8/15	11/19/15	12	Gonzalez	518.81
6	55801	Ferrari	Sidney	2008-04-05	F	11/10/15	11/21/15	12	Gonzalez	493.02

This doesn't look very different, but note the subtle change in what the dates look like in the birthdate column. This is simply how Datetime objects are written out. Now we can calculate ages. The easiest way is to figure out how many years are between the birthdate and the current date. There is a function that gives us the current date and time:

In [18]:
```
pd.datetime.now()
```

Out[18]:
```
datetime.datetime(2018, 4, 16, 15, 51, 5, 458866)
```

What's returned in the parentheses is the current date and time, from largest quantity to the smallest (the final number is the number of microseconds!). With the following expression, we can create a new column called `age` in the data frame, calculating the difference between the current date and each birthdate, and then taking the year part of what is left over. When we print `patients` again, we can see the new column at the end.

In [19]:
```
patients["age"] = (pd.datetime.now() - patients["birthdate"]).astype("timedelta64
patients
```

Out[19]:

	patientid	lastname	firstname	birthdate	sex	admit	discharge	los	physician	dx1	age
0	55421	Blaine	Richard	2012-01-05	M	11/30/15	12/30/15	31	Anderson	300.01	6
1	55426	Lazlo	Ilsa	2010-07-06	F	11/10/15	11/21/15	12	Anderson	518.81	7
2	55427	Lazlo	Victor	2007-05-13	M	11/2/15	11/3/15	2	Jones	493.22	10
3	55983	Renault	Louis	2004-03-25	M	11/1/15	11/2/15	2	Jones	518.81	14
4	55678	Strasser	Heinrich	2007-04-30	M	11/4/15	11/5/15	2	Gonzalez	493.02	10
5	55900	Ugarte	Peter	2013-01-05	M	11/8/15	11/19/15	12	Gonzalez	518.81	5
6	55801	Ferrari	Sidney	2008-04-05	F	11/10/15	11/21/15	12	Gonzalez	493.02	10

Let's now turn to the NHANES data set. There are 10,175 observations in this data set. If we just typed `nhanes` , the notebook would be smart enough not to print them all, but it would still print quite a few of them. We can use the `head()` function to just get the first few observations to see the general structure:

In [20]:
```
nhanes.head()
```

Out[20]:

	id	sex	age	ethnicity	edu	income	height	weight	bmi	systolic	diastolic
0	73557.0	Male	69	Black	HS grad/GED	$15K-20K$ <	171.3	78.3	26.7	122.0	72.0
1	73558.0	Male	54	White	HS grad/GED	$35K-45K$ <	176.8	89.5	28.6	156.0	62.0
2	73559.0	Male	72	White	Some college/AA	$65K-75K$ <	175.3	88.9	28.9	140.0	90.0
3	73560.0	Male	9	White	NaN	$55K-65K$ <	137.3	32.2	17.1	108.0	38.0
4	73561.0	Female	73	White	College graduate or above	$100K+	162.4	52.0	19.7	136.0	86.0

This data consists of an ID number, the sex, age, ethnicity, education and income levels of the participants, as well as some clinical data. You can probably guess what many of them are:

- height

- weight
- body-mass index (our old friend!)
- systolic and diastolic blood pressure
- high- and low-density lipoproteins (*i.e.*, "good" and "bad" cholesterol)
- total cholesterol (includes more than just HDL and LDL levels)
- triglycerides (another measure of lipid levels)
- blood glucose
- number of cigarettes smoked in the last 30 days

The full NHANES data set includes literally hundreds of variables measured for each person, so this is only a tiny portion. Note that not all information is recorded for all participants. In Pandas, the convention is to put `NaN` (Not-a-Number) as a flag for missing data.

Let's suppose that we want to filter the data so that only patients 18 years of age and older are included. This is easy to do in Pandas. Again, the operations are vectorized, and there is no need to create loops:

In [21]:
```
nhanes_adults = nhanes[nhanes["age"] >= 18]
nhanes_adults.head()
```

Out[21]:

	id	sex	age	ethnicity	edu	income	height	weight	bmi	systolic	diastolic
0	73557.0	Male	69	Black	HS grad/GED	$15K-$20K $<$	171.3	78.3	26.7	122.0	72.0
1	73558.0	Male	54	White	HS grad/GED	$35K-$45K $<$	176.8	89.5	28.6	156.0	62.0
2	73559.0	Male	72	White	Some college/AA	$65K-$75K $<$	175.3	88.9	28.9	140.0	90.0
4	73561.0	Female	73	White	College graduate or above	\$100K+	162.4	52.0	19.7	136.0	86.0
5	73562.0	Male	56	Mexican American	Some college/AA	$55K-$65K $<$	158.7	105.0	41.7	160.0	84.0

We can do some rather sophisticated things with this data using Pandas, things that we usually require a stats package, or perhaps Microsoft Excel, to do. The following calculates the average values, by sex, for the numerical columns in the data. Note that taking the mean of `id` isn't very helpful, but it is a numeric column, so was included in the command.

In [22]:
```
nhanes_adults.groupby("sex").mean()
```

Out[22]:

	id	age	height	weight	bmi	systolic	diastolic	h
sex								
Female	78662.207382	47.468251	160.472747	75.985794	29.445386	120.476973	68.357015	57.1038
Male	78709.447874	47.294582	174.329095	86.445961	28.342350	124.558476	70.606476	47.9400

We can calculate such statistics on multiple levels. The following shows means within each sex, and also within each ethnic group:

In [23]:
```
nhanes_adults.groupby(["ethnicity", "sex"]).mean()
```

Out[23]:

		id	age	height	weight	bmi	systolic	
ethnicity	**sex**							
Black	**Female**	78677.978261	45.986025	162.747280	84.370305	31.845586	123.630824	6
	Male	78701.285246	48.042623	176.364463	89.708007	28.743590	128.314286	7
Mexican American	**Female**	78618.874429	43.292237	157.025829	75.725943	30.630095	118.304462	6
	Male	78698.139024	44.987805	170.470483	85.859033	29.457761	124.360111	7
Other Hispanic	**Female**	78945.153595	46.111111	158.106463	72.535714	28.974403	119.492857	6
	Male	78441.598291	45.854701	171.032743	83.142035	28.292478	124.162679	6
Other/Multiracial	**Female**	78806.765458	44.373134	157.855204	63.925566	25.561312	117.509901	6
	Male	78696.450116	44.111369	171.398768	76.985679	26.068395	123.139108	7
White	**Female**	78553.583582	50.938806	161.947068	76.948710	29.335266	120.937182	6
	Male	78772.725426	49.080422	176.236416	88.883993	28.561591	123.294434	7

A slightly different command gives us the mean for just one column, BMI. Since it's just one column, the notebook interface doesn't convert it to a nice table, but it's easy enough to read.

In [24]:
```
pd.pivot_table(nhanes_adults, "bmi", "sex")
```

Out[24]:

	bmi
sex	
Female	29.445386
Male	28.342350

We can use the same command for multi-level tables as well. Here is BMI by sex and ethnicity:

```
In [25]: pd.pivot_table(nhanes_adults, "bmi", "ethnicity", "sex")
```

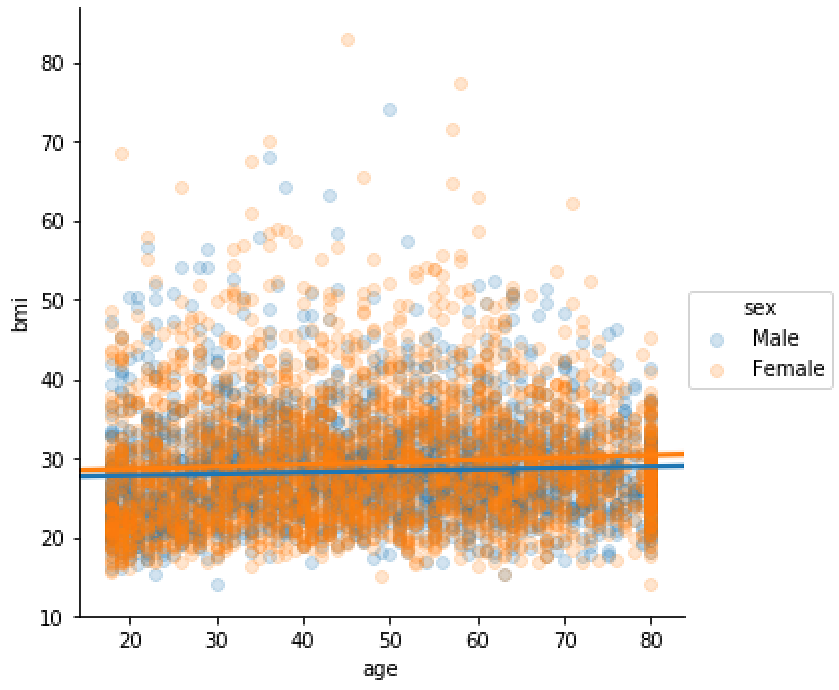
```
Out[25]:
```

sex	Female	Male
ethnicity		
Black	31.845586	28.743590
Mexican American	30.630095	29.457761
Other Hispanic	28.974403	28.292478
Other/Multiracial	25.561312	26.068395
White	29.335266	28.561591

Finally, let's create a plot of all the adult BMIs, with age on the *x*-axis, and BMI on the *y*-axis. We'll give males and females different colors. Since there are so many points, we will make them partially transparent, so that it's not a big wall of color. This is what the `alpha` in the command means: make the points 20% opaque (0% would make them completely transparent, and thus invisible!). While we can do this in Matplotlib, the Seaborn package has a number of enhancements to make statistical plots like these easier to express. Much as Pandas is written on top of NumPy, Seaborn is written on top of Matplotlib.

The particular command below also draws separate linear regression fits to the data for males and females, to see the overall trends. I admit that I don't yet know how to make a Seaborn plot any bigger on the notebook interface (I've tried), so I apologize for the small size!

```
In [26]: scatterplot = sns.lmplot(x="age", y="bmi", hue="sex", data=nhanes_adults, scatter
```



This walkthrough should give you a hint of what is available via packages like NumPy, Pandas, Matplotlib, and Seaborn. They don't have all the features of a full statistical package like R, but you may now have an idea of why Python has become so popular in the sciences as a language to work with data. The notebook interface of Jupyter (https://jupyter.org/) (formerly called iPython Notebook (http://ipython.org/)) is a significant bonus, too, as it allows programmers to save work, results, plots, and commentary all in one document.

Be sure to take a look at the lecture notes for this week for more information, as well as the course Moodle site, which will have links to documentation and downloads for these and other packages. I hope this brief demonstration has piqued your interest!

Dave...

```
In [ ]:
```

```
In [ ]:
```