STAT221Week09

STAT 221 Week 9: Markov Chains

STAT 221 2010 S1: Monte Carlo Methods

Markov chain, named after Andrey Markov, is a mathematical model for a possibly dependent sequence of random variables. Intuitively, a Markov Chain is a system which "jumps" among several states, with the next state depending (probabilistically) only on the current state. A useful heuristic is that of a frog jumping among several lily-pads, where the frog's memory is short enough that it doesn't remember what lily-pad it was last on, and so its next jump can only be influenced by where it is now.

Formally, the Markov property states that the conditional probability distribution for the system at the next step (and in fact at all future steps) *given* its current state depends only on the current state of the system, and not additionally on the state of the system at previous steps:

$$P(X_{n+1}|X_1,X_2,\ldots,X_n) = P(X_{n+1}|X_n).$$

Since the system changes randomly, it is generally impossible to predict the exact state of the system in the future. However, the statistical and probailistic properties of the system's future can be predicted. In many applications it is these statistical properties that are important.

Formal definition and terms

A **Markov chain** is a sequence of random variables $X_1, X_2, X_3, \ldots$ with the **Markov property**, namely that, given the present state, the future and past states are independent. Formally,

$$P(X_{n+1}=x|X_1=x_1,X_2=x_2\ldots,X_n=x_n) = P(X_{n+1}=x|X_n=x_n).$$

The possible values of X_i or the set of all states of the system form a countable set $\mathbb{X}$ called the **state space** of the chain.

The changes of state of the system are called **transitions**, and the probabilities associated with various state-changes are called **transition probabilities**.

Markov chains are often depicted by a weighted directed graph, where the edges are labeled by the probabilities of going from one state to the other states. This is called the **flow diagram** or **transition probability diagram**. The **transition probability matrix** $\mathbf{P}$ encodes the probabilities associated with state-changes or "jumps" from one state to another in the state-space $\mathbb{X}$. If $\mathbb{X}$ is labelled by $\{0,1,2,\ldots\}$ then the i,j-th entry in the matrix $\mathbf{P}$ corresponds to the probability of going from state i to state j in one time-step.

$$\mathbf{P} = \begin{bmatrix} p_{0,0} & p_{0,1} & p_{0,2} & \cdots \\ p_{1,0} & p_{1,1} & p_{1,2} & \cdots \\ p_{2,0} & p_{2,1} & p_{2,2} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

The state of the system at the n-th time step is described by a **state probability vector**

$$\mathbf{p}^{(n)} = \left(\mathbf{p}_0^{(n)}, \mathbf{p}_1^{(n)}, \mathbf{p}_2^{(n)}, \ldots\right)$$

Thus, $\mathbf{p}_i^{(n)}$ is the probability you will find the Markov chain at state $i \in \mathbb{X}$ at time-step n and

$\mathbf{p}_i^{(0)}$ is called the **initial probability vector** at the convenient initial time 0.

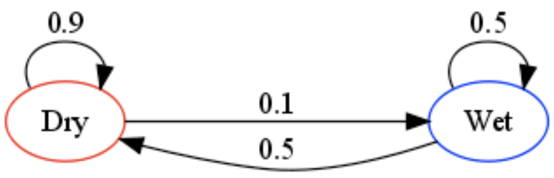
The state space $\mathbb{X}$ and transition probability matrix $\mathbf{P}$ completely characterizes a Markov chain.

Example 1: Dry-Wet chain, a toy weather model - Sage break-down of the Wiki Example

We can coarsely describe the weather of a given day by a toy model that states if it is "wet" or "dry". Each day the weather in our toy model is an element of our state space

$$\mathbb{X} = \{\text{"wet"}, \text{"dry"}\}.$$

We can make a picture of our toy probability model with a flow diagram or transition probability diagram as follows:



The probabilities of weather conditions, given the weather on the preceding day, can be represented by a transition probability matrix:

$$\mathbf{P} = \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix}$$

The matrix $\mathbf{P}$ represents our toy weather model in which a dry day is 90% likely to be followed by another dry day, and a wet or rainy day is 50% likely to be followed by another wet day. The columns can be labelled "dry" and "wet" respectively, and the rows can be labelled in the same manner. For convenience, we will use integer labels 0 and 1 for "dry" and "wet", respectively.

$(\mathbf{P})_{ij} = p_{i,j}$ is the probability that, if a given day is of type i, it will be followed by a day of type j.

Since the transition probability matrix $\mathbf{P}$ is a **stochastic matrix**:

- The rows of $\mathbf{P}$ sum to 1.
- The probabiltites in each row can be thought of as "current-state" specific $de\ Moivre(p'_{i,j}s)$ disritbution
- Basically, you toss a current-state-specific many-faced weigted die to determine the next state
- How can we think of our toy weather model in terms of two Bernouli trials; $Bernoulli(0.9)$ and $Bernoulli(0.5)$? -- recall a fair coin in the wet pocket and the biased coin in the dry pocket analogy from lectures...

How do we represent a matrix $\mathbf{P}$ in Sage?

```
help(matrix)
```

docs-0.html

```
P = matrix(RR,[[9/10,1/10],[1/2,1/2]])  # construct and assign
```

```
the matrix to P
# could have used QQ instead of RR above if the probs are
rational and for exact rational arithmetic
P                                       # display P
```

```
    [0.900000000000000 0.100000000000000]
    [0.500000000000000 0.500000000000000]
```

```
P[0,1]                                  # accessing (i,j)-th
entry of matrix P
```

```
# know the parent of your matrix type, especially if you are a
Math/Stat major
P.parent()
```

Predicting the weather with our Dry-Wet chain

The weather on day 0 is known to be dry. This is represented by a probability vector in which the "dry" entry is 100%, and the "wet" entry is 0%:

$$\mathbf{p}^{(0)} = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

The weather on day 1 can be predicted by:

$$\mathbf{p}^{(1)} = \mathbf{p}^{(0)}\,\mathbf{P} = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix} = \begin{bmatrix} 0.9 & 0.1 \end{bmatrix}$$

Thus, there is an 90% chance that day 1 will also be sunny.

```
p0 = vector((1,0))    # initial probability vector for a dry day
zero
p0
```

```
p1 = p0*P                    #
p1
```

```

```

The weather on day 2 can be predicted in the same way:

$$\mathbf{p}^{(2)} = \mathbf{p}^{(1)}\,\mathbf{P} = \mathbf{p}^{(0)}\,\mathbf{P}^2 = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix}^2 = \begin{bmatrix} 0.86 & 0.14 \end{bmatrix}$$

or, equivalently,

$$\mathbf{p}^{(2)} = \mathbf{p}^{(1)}\,\mathbf{P} = \begin{bmatrix} 0.9 & 0.1 \end{bmatrix} \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix} = \begin{bmatrix} 0.86 & 0.14 \end{bmatrix}$$

How do we do this in Sage?

```
p2 = p0*P^2       # left multiply the initial probability vector
by square of P
p2                # disclose the probability vector at time-step
2
```

or, equivalently,

```
p2 = p1*P         # left multiply the probability vector at
time-step 1 by P
# disclose the probability vector at time-step 2 (compare output
of previous cell)
p2
```

General rules for day $n$ follow from mathematical induction are:

$$\mathbf{p}^{(n)} = \mathbf{p}^{(n-1)}\,\mathbf{P}$$

$$\mathbf{p}^{(n)} = \mathbf{p}^{(0)}\,\mathbf{P}^{n}$$

How do we operate with a matrix in Sage to do this for any given $n$?

```
n = 3                       # assign some specific time-step or
day
dry_p0 = vector((1,0))      # initial probability vector for a dry
day zero
pn = dry_p0 * P^n           # probability vector for day n
pn                          # display it
```

```
n = 3                       # assign some specific time-step or
day
wet_p0 = vector((0,1))      # initial probability vector for a wet
day zero
pn = wet_p0 * P^n           # probability vector for day n
pn                          # display it
```

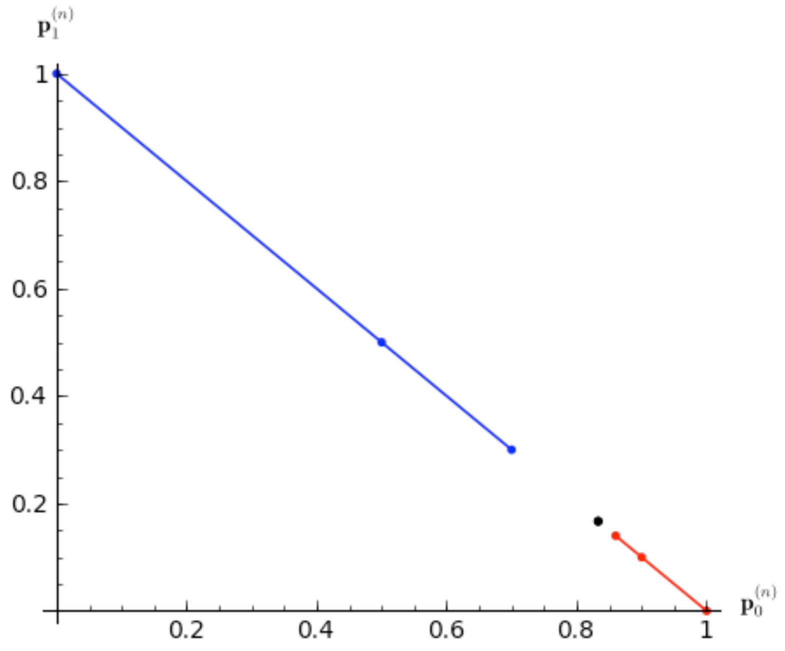
```
nmax = 3              # maximum number of days or time-steps of
interest
[(n, vector((0,1)) * P^n ) for n in range(nmax+1)] # state
probability vector at time n=0,1,...,nmax
```

```
%hide
# what's going on here...  try to increase nmax and see where
the state prob vector is going
nmax=2  # maximum number of time-steps of interest
# the next line is just html figure heading
html("<h3>$n$-step state probability vector
$\mathbf{p}^{(n)}=(\mathbf{p}^{(n)}_0,\mathbf{p}^{(n)}_1)$,
$n=0,1,\ldots,$ %s steps</h3>"%nmax)
# now we will plot the prob vectors
# the red points start on a dry day 0
pns_plot = point([vector((1,0)) * P^n  for n in
range(nmax+1)],color='red')
pns_plot += line([vector((1,0)) * P^n  for n in
range(nmax+1)],color='red')
# the blue points start on a wet day 0
pns_plot += point([vector((0,1)) * P^n  for n in
range(nmax+1)],color='blue')
pns_plot += line([vector((0,1)) * P^n  for n in
range(nmax+1)],color='blue')
# suppose we had initial state prob vector (0.833,0.167) then
where do we go
pns_plot += point([vector((0.833,0.167)) * P^n  for n in
range(nmax+1)],color='black')
```

```
pns_plot += line([vector((0.833,0.167)) * P^n  for n in
range(nmax+1)],color='black')
pns_plot.show(figsize=[5,4],

axes_labels=['$\mathbf{p}^{(n)}_0$','$\mathbf{p}^{(n)}_1$'])
```

n-step state probability vector $\mathbf{p}^{(n)} = (\mathbf{p}_0^{(n)}, \mathbf{p}_1^{(n)}), \quad n = 0, 1, .$



Steady state of the weather in our Dry-Wet chain

In this example, predictions for the weather on more distant days are increasingly inaccurate and tend towards a steady state vector. This vector represents the probabilities of dry and wet weather on all days, and is independent of the initial weather.

The steady state vector is defined as:

$$\mathbf{s} = \lim_{n \to \infty} \mathbf{p}^{(n)}$$

but only converges to a strictly positive vector if $\mathbf{P}$ is a **regular** transition matrix (that is, there is at least one $\mathbf{P}^n$ with all non-zero entries making the Markov chain **irreducible** and **aperiodic**).

Since the $\mathbf{s}$ is independent from initial conditions, it must be unchanged when transformed by $\mathbf{P}$. This makes it an **eigenvector** (with **eigenvalue** 1), and means it can be derived from $\mathbf{P}$. For our toy model of weather:

$$\begin{aligned}
\mathbf{P} &= \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix} \\
\mathbf{s}\,\mathbf{P} &= \mathbf{s} \qquad (\mathbf{s} \text{ is unchanged by } \mathbf{P}.) \\
&= \mathbf{s}\,\mathbf{I} \\
\mathbf{s}\,(\mathbf{P}-\mathbf{I}) &= \mathbf{0} \\
&= \mathbf{s}\left(\begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) \\
&= \mathbf{s}\begin{bmatrix} -0.1 & 0.1 \\ 0.5 & -0.5 \end{bmatrix}
\end{aligned}$$

$$\begin{bmatrix} \mathbf{s}_0 & \mathbf{s}_1 \end{bmatrix} \begin{bmatrix} -0.1 & 0.1 \\ 0.5 & -0.5 \end{bmatrix} = \begin{bmatrix} 0 & 0 \end{bmatrix}$$

So $-0.1\mathbf{s}_0 + 0.5\mathbf{s}_1 = 0$ and since they are a probability vector we know that $\mathbf{s}_0 + \mathbf{s}_1 = 1$.

Solving this pair of simultaneous equations gives the steady state distribution:

$$(\mathbf{s}_0, \mathbf{s}_1) = (5/6, 1/6) = (0.833, 0.167)$$

In conclusion, in the long term, 83% of days are dry.

How do we operate the above to solve for $\mathbf{s}$ in Sage? There are two "methods". We can either use

- Method 1: solve a system of linear equations with solve to get $\sim$ or
- Method 2: obtain $\mathbf{s}$ via eigen decomposition.

You are not expected to follow method 2 if you have not had been introduced to eigen values and eigen vectors.

Method 1: Solving a system of equations to obtain $\sim$.

```
#P = matrix(QQ,[[9/10,1/10],[1/2,1/2]]); P; P.parent()
P = matrix(RR,[[9/10,1/10],[1/2,1/2]]); P; P.parent()
```

```
I=matrix(2,2,1); I; I.parent()      # the 2X2 identity matrix
```

```
P-I; (P-I).parent()
```

```
s0, s1 = var('s0, s1')
```

```
eqs = vector((s0,s1)) * (P-I); eqs[0]; eqs[1]
```

```
solve([eqs[0] == 0, eqs[1]==0, s0+s1==1], s0,s1)
```

```
solve([eqs[0] == 0, s0+s1==1], s0,s1)        # just use
eqs[0]==0 since eqs[1]==0 is redundant
```

```
solve([eqs[1]==0, s0+s1==1], s0,s1)          # just use
eqs[1]==0 since eqs[0]==0 is redundant
```

End of Method 1 to solve for the steady state vector **s**.

Method 2: Alternatively use eigen decomposition over rationals in Sage to solve for $\sim$. You may ignore this if you hove not seen eigen decomposition before. To follow Method 2 you need to know a bit more about eigen values, eigen vectors and eigen spaces if you are interested.

```
P = matrix(QQ,[[9/10,1/10],[1/2,1/2]]); P; P.parent()
```

```
P.eigenvalues()
```

```
D, V = P.eigenmatrix_left()   # left eigen decomposition
D                             # diagonal matrix of eigen values
```

```
V                             # left eigen vectors
```

```
# checking when we left-multiply by left-eigenvector
# of eigenvalue 1 we get the output scaled by 1
V[0]; V[0]*P
```

```
# checking when we left-multiply by left-eigenvector
# of eigenvalue 2/5 we get the output scaled by 2/5
V[1]; V[1]*P
```

```
V.inverse()*D*V
```

```
# checking that the eigen decomposition of P is indeed P
V*D*V.inverse()
```

```
EigVecForEigValue1 = V[0]; EigVecForEigValue1
```

```
EigVecForEigValue1.norm(1)  # normalization factor
```

```
# normalize to make it a probability vector
EigVecForEigValue1 / EigVecForEigValue1.norm(1)
```

```

```

End of Method 2.

Rainfall Data in Christchurch

Paul Brouwers has a basic CliFlo datafeed on

http://www.math.canterbury.ac.nz/php/lib/cliflo/?range=20100425:20100501

This returns the date and rainfall in mm as measured from the CHCH aeroclub station. It is assumed that days without readings would not be listed. It expects a range parameter such as: ?range=20100425:20100501 The first number is the starting search date (YYYYMMDD). Colon as separator. The first number is the ending search date (YYYYMMDD). CliFlo limits us to 2 million rows for the subscription and 40,000 rows per query (which is equivalent of over 100 years of data, so I we're safe - The data doesn't go back much before 1944).

```
%auto
import urllib2 as U
#wetdataURL = 'http://www.math.canterbury.ac.nz/php/lib/cliflo/?
range=20100101:20100510'
wetdataURL =
'http://www.math.canterbury.ac.nz/php/lib/cliflo/rainfall.php'
wetdata = U.urlopen(wetdataURL).readlines()
datalines=[]
for a_line in wetdata:
    #print a_line
    temp = a_line.replace('\n','').split(',')
    temp = [float(q) for q in temp if q != ',']
    datalines.append(temp)
```

```
datalines[0]
```

```
    [19430802.0, 0.0]
```

```
len(datalines)
```

```
    24212
```

```
(2010-1943)*365
```

```
    24455
```

```
@interact
def chch_precipitation(start_date = slider(0,len(datalines)-
1,1,len(datalines)-100), end_date = slider(0,len(datalines)-
1,1,len(datalines)-1)):
    htmls1 = '<h3>Daily Precipitation at Christchurch, fed from
NIWA data</h3>'
    html(htmls1+"<h4>from
%s</h4>"%int(datalines[start_date][0])+"<h4>until
%s</h4>"%int(datalines[end_date][0]))
    sel_data = datalines[start_date:end_date]
    c_max = max([q[1] for q in sel_data])
    c_min = min([q[1] for q in sel_data])
    sel_daysdata = [[i,sel_data[i][1]] for i in
range(len(sel_data))]
    show(list_plot(sel_daysdata, plotjoined=True,
rgbcolor=(0,0,1)) , ymin = c_min-2, axes = True, ymax = c_max+3,
frame = False, axes_labels=['days', 'mm'])
```

```
xx=datalines[200:210]; xx
```

```
[xx[i][1] for i in range(len(xx))]
```

```
[xx[i][1]>0 for i in range(len(xx))]
```

```
[int(xx[i][1]>0) for i in range(len(xx))]
```

Grab all the days data from start to end:

```
%auto
all_daysdata = [[i,int(datalines[i][1]>0)] for i in
range(len(datalines))] # all the data as 0s and 1s
```

Interactive cell to allow you to select some specific data and turn it into the list of 0 or 1 tuples (this list will then be available in `sel_daysdata` in later cells in the worksheet).

```
@interact
def chch_wetdry(output = checkbox(False, "Print out selected
Data?"),start_date = slider(0,len(datalines)-1,1,len(datalines)-
100), end_date = slider(0,len(datalines)-1,1,len(datalines)-1)):
    htmls1 = '<h3>Daily Precipitation at Christchurch, fed from
NIWA data</h3>'
    html(htmls1+"<h4>from
%s</h4>"%int(datalines[start_date][0])+"<h4>until
%s</h4>"%int(datalines[end_date][0]))
    global sel_daysdata  # made it a global so it is easy to
choose data
    sel_data = datalines[start_date:end_date]
    sel_daysdata = [[i,int(sel_data[i][1]>0)] for i in
range(len(sel_data))]
    show(list_plot(sel_daysdata, plotjoined=True,
rgbcolor=(0,0,1)) , ymin = 0, axes = True, ymax = +1, frame =
False, axes_labels=['days', 'wet/dry'])
    if(output):
        print sel_daysdata
```

```
sel_daysdata
```

```
x0ton = [sel_daysdata[i][1] for i in range(len(sel_daysdata))]
x0ton
```

```
len(x0ton)
```

Maximum likelihood estimation of the unknown transition probabilities for the Dry-Wet Markov chain model of Christchurch weather

In the example we have been working with earlier, the transition probabilities were given by the matrix

$$\mathbf{P} = \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix}$$

and we simply used the given $\mathbf{P}$ to understand the properties and utilities of the probability model for a possibly dependent sequence of $\{0,1\}$-valued random variables encoding the $\{\mathrm{Dry}, \mathrm{Wet}\}$ days, respectively.

What we want to do now is use the data from Christchurch's Aeroclub obtained from NIWA to **estimate** Christchurch's unknown transition probability matrix

$$\mathbf{P} = \begin{bmatrix} p_{0,0} & p_{0,1} \\ p_{1,0} & p_{1,1} \end{bmatrix}.$$

Let us use the principle of maximum likelihood and derive the maximum likelihood estimator

$$\widehat{\mathbf{P}} = \begin{bmatrix} \hat{p}_{0,0} & \hat{p}_{0,1} \\ \hat{p}_{1,0} & \hat{p}_{1,1} \end{bmatrix}.$$

Recall that the likelihood function

$$L(\text{unknown parameters ; Data})$$

is essentially the joint density of the data $X_0, X_1, X_2, \ldots, X_n$ as a function of the parameters. The data gives $n+1$ consecutive days of Dry or Wet recordings as 0 or 1 at the Christchurch's Aeroclub. What are the unknown parameters here? Well, they are the four entries $(p_{0,0}, p_{0,1}, p_{1,0}, p_{1,1})$ of the unknown $\mathbf{P}$. But, due to the fact that $\mathbf{P}$ is not any old matrix of real numbers, but rather a stochastic matrix, it is constrained so that the entries are non-negative and the entries of each row sums to 1. For instance we can write the off-diagonal entries in terms of the diagonal entries $p_{0,1} = 1 - p_{0,0}$ and $p_{1,0} = 1 - p_{1,1}$ and merely treat two parameters $(p_{0,0}, p_{1,1})$ as the truly unknowns that can take any value in the unit square $[0,1] \times [0,1]$ parameter space.

$$\begin{aligned} L(p_{0,0}, p_{1,1}) &= L(p_{0,0}, p_{1,1}; x_0, x_1, \ldots, x_n) \\ &= P\left(X_0 = x_0, X_1 = x_1, \ldots, X_{n-1} = x_{n-1}, X_n = x_n\right) \end{aligned}$$

In the above equation, we are given that the transition probabilities are $p_{0,0}, p_{1,1}$. Now, by definition of conditional probability and the markov property,

$$\begin{aligned} L(p_{0,0}, p_{1,1}) &= P\left(X_n = x_n \mid X_{n-1} = x_{n-1}, \ldots, X_2 = x_2, X_1 = x_1, X_0 = x_0\right) P\left(X_{n-1} = x_{n-1}, \ldots, X_2 = x_2, X_1 = x_1, X_0 = x_0\right) \\ &= P\left(X_n = x_n \mid X_{n-1} = x_{n-1}\right) P\left(X_{n-1} = x_{n-1}, \ldots, X_2 = x_2, X_1 = x_1, X_0 = x_0\right) \\ &= P\left(X_n = x_n \mid X_{n-1} = x_{n-1}\right) P\left(X_{n-1} = x_{n-1} \mid X_{n-2} = x_{n-2}, X_{n-3} = x_{n-3}, \ldots, X_2 = x_2, X_1 = x_1, X_0 = x_0\right) \\ &\qquad P\left(X_{n-2} = x_{n-2}, X_{n-3} = x_{n-3}, \ldots, X_2 = x_2, X_1 = x_1, X_0 = x_0\right) \\ &= P\left(X_n = x_n \mid X_{n-1} = x_{n-1}\right) P\left(X_{n-1} = x_{n-1} \mid X_{n-2} = x_{n-2}\right) P\left(X_{n-2} = x_{n-2}, X_{n-3} = x_{n-3}, \ldots, X_2 = x_2, X_1 = x_1, X_0 = x_0\right) \\ &\vdots \\ &= P\left(X_n = x_n \mid X_{n-1} = x_{n-1}\right) P\left(X_{n-1} = x_{n-1} \mid X_{n-2} = x_{n-2}\right) \cdots P\left(X_2 = x_2 \mid X_1 = x_1\right) P\left(X_1 = x_1 \mid X_0 = x_0\right) P\left(X_0 = x_0\right) \\ &= P\left(X_0 = x_0\right) \prod_{i=1}^{n} P\left(X_i = x_i \mid X_{i-1} = x_{i-1}\right) \\ &= \left(p_{0,0}\right)^{n_{0,0}} \left(1 - p_{0,0}\right)^{n_{0,1}} \left(p_{1,1}\right)^{n_{1,1}} \left(1 - p_{1,1}\right)^{n_{1,0}}, \end{aligned}$$

where, $n_{i,j}$ is the number of transitions from state i to state j in the observed data sequence $x_0, x_1, \ldots, x_n$. Therefore the log likelihood function is

$$\begin{aligned} l(p_{0,0}, p_{1,1}) &= \log\left(L(p_{0,0}, p_{1,1})\right) \\ &= \log\left(\left(p_{0,0}\right)^{n_{0,0}} \left(1 - p_{0,0}\right)^{n_{0,1}} \left(p_{1,1}\right)^{n_{1,1}} \left(1 - p_{1,1}\right)^{n_{1,0}}\right) \\ &= n_{0,0} \log\left(p_{0,0}\right) + n_{0,1} \log\left(1 - p_{0,0}\right) + n_{1,1} \log\left(p_{1,1}\right) + n_{1,0} \log\left(1 - p_{1,1}\right) \end{aligned}$$

Finally, we can find the maximum likelihood estimates (MLEs) $\widehat{p}_{0,0}$ and $\widehat{p}_{1,1}$ for the unknown transition probabilities $p_{0,0}$ and $p_{1,1}$ by differentiating the loglikelihood function with respect to

$p_{0,0}$ and $p_{1,1}$, respectively, and solving the resulting equations in terms of the variable of differentiation. This will yield the following which me can also obtain symbolically in sage.

$$\begin{aligned}\frac{d}{dp_{0,0}}\left(l(p_{0,0},p_{1,1})\right) &= \frac{d}{dp_{0,0}}\left(n_{0,0}\log\left(p_{0,0}\right)+n_{0,1}\log\left(1-p_{0,0}\right)+n_{1,1}\log\left(p_{1,1}\right)+n_{1,0}\log\left(1-p_{1,1}\right)\right)\\ &= \dots\\ &= \frac{n_{0,0}}{p_{0,0}}-\frac{n_{0,1}}{1-p_{0,0}}\end{aligned}$$

Similarly,

$$\begin{aligned}\frac{d}{dp_{1,1}}\left(l(p_{0,0},p_{1,1})\right) &= \frac{d}{dp_{1,1}}\left(n_{0,0}\log\left(p_{0,0}\right)+n_{0,1}\log\left(1-p_{0,0}\right)+n_{1,1}\log\left(p_{1,1}\right)+n_{1,0}\log\left(1-p_{1,1}\right)\right)\\ &= \dots\\ &= \frac{n_{1,1}}{p_{1,1}}-\frac{n_{1,0}}{1-p_{1,1}}\end{aligned}$$

Finally, solving the above equations in terms of $p_{0,0}$ and $p_{1,1}$ gives the MLEs that

$$\widehat{p}_{0,0}=\frac{n_{0,0}}{n_{0,0}+n_{0,1}} \quad \text{and} \quad \widehat{p}_{1,1}=\frac{n_{1,1}}{n_{1,0}+n_{1,1}}$$

as follows:

$$\begin{aligned}\frac{d}{dp_{0,0}}\left(l(p_{0,0},p_{1,1})\right) &= 0\\ &\Leftrightarrow \frac{n_{0,0}}{p_{0,0}}-\frac{n_{0,1}}{1-p_{0,0}}=0\\ &\Leftrightarrow p_{0,0}=\frac{n_{0,0}}{n_{0,0}+n_{0,1}}\end{aligned}$$

and

$$\begin{aligned}\frac{d}{dp_{1,1}}\left(l(p_{0,0},p_{1,1})\right) &= 0\\ &\Leftrightarrow \frac{n_{1,1}}{p_{1,1}}-\frac{n_{1,0}}{1-p_{1,1}}=0\\ &\Leftrightarrow p_{1,1}=\frac{n_{1,1}}{n_{1,0}+n_{1,1}}\end{aligned}$$

```
%auto
var('p00, p11, n00, n01, n10, n11') # declare variables
# assign the symbolic expression for the log likelihood function
to L
L=n00*log(p00) + n01*log(1-p00) + n11*log(p11) + n10*log(1-p11)
```

```
L.diff(p00)  # differentiate log likelihood symbolically with
respect to p00
```

```
    n01/(p00 - 1) + n00/p00
```

```
L.diff(p11)  # differentiate log likelihood symbolically with
respect to p11
```

```
    n10/(p11 - 1) + n11/p11
```

```
solve(L.diff(p00)==0, p00)  # solve the equation in terms of p00
to get MLE
```

```
    [p00 == n00/(n00 + n01)]
```

```
solve(L.diff(p11)==0, p11)  # solve the equation in terms of p11
to get MLE
```

```
    [p11 == n11/(n10 + n11)]
```

```
x0ton = [sel_daysdata[i][1] for i in range(len(sel_daysdata))]
transitions_data =[(x0ton[i],x0ton[i+1]) for i in
range(0,len(x0ton)-1,1)]
#transitions_data
```

```
transition_counts = makeFreqDict(transitions_data)
transition_counts
```

```
n_00 = transition_counts[(0,0)]
n_01 = transition_counts[(0,1)]
n_10 = transition_counts[(1,0)]
n_11 = transition_counts[(1,1)]
n_00, n_01, n_10, n_11
```

Make a function to make a transition counts matrix from any list of 0/1 tuples passed in.

```
%auto
def makeTransitionCounts(theData):
    '''Return a transition counts matrix from a list of tuples
representing transitions between 2 states 0 and 1.

    Param theData is a list of tuples where the tuples can be
(0,0) or (0,1) or (1,0) or (1,1).
    Return a 2x2 matrix [[count of (0,0), count of (0,1)],[count
of (1,0), count of (1,1)]].'''

    retMatrix = matrix([[0,0],[0,0]]) # default counts
    x0ton = [theData[i][1] for i in range(len(theData))]
    transitions_data =[(x0ton[i],x0ton[i+1]) for i in
range(0,len(x0ton)-1,1)]
    transition_counts = makeFreqDict(transitions_data)
    #keysToFind = [(0,0),(0,1),(1,0),(1,1)]
    # we will get an error if we try to access a value for a key
that is not in the dictionary
    # so we need to check if each of the keys we might find is
in the dictionary
    # and only try to access the count if the key is there
    for i in [0,1]:
        for j in [0,1]:
            if (i,j) in transition_counts:
                retMatrix[i,j] = transition_counts[(i,j)]
            # else the value in the matrix [i,j] stays as 0
    return retMatrix
```

Get the transition counts matrix for all the data (we will get the same as we had before, but as a matrix which echoes the layout of our transition probabilities matrix, and we would also be able to use our function for other lists of tuples):

```
allTransitionCounts = makeTransitionCounts(all_daysdata)
allTransitionCounts
```

Make a function to turn transitions counts into a matrix of values for $\widehat{\mathbf{P}} = \begin{bmatrix} \hat{p}_{0,0} & \hat{p}_{0,1} \\ \hat{p}_{1,0} & \hat{p}_{1,1} \end{bmatrix}$.

```
%auto
def makeMLEMatrix(tcMatrix):
    '''Return an MLE Matrix from given 2-state transition count
data.

    Param tcMatrix is a 2x2 matrix of transition counts.
    Returns MLE matrix as
    [[n_00/(n_00+n_01), n_01/(n_00+n_01)], [n_10/(n_10+n_11),
n_11/(n_10+n_11)]].
    Returns None if there is not at least one count in each row
of tcMatrix.'''

    retValue = None
    if (tcMatrix[0] > 0) and (tcMatrix[1] > 0):
        retValue =
matrix(RR,[[tcMatrix[0,0]/(tcMatrix[0,0]+tcMatrix[0,1]),
tcMatrix[0,1]/(tcMatrix[0,0]+tcMatrix[0,1])],[tcMatrix[1,0] /
(tcMatrix[1,0]+tcMatrix[1,1]),
tcMatrix[1,1]/(tcMatrix[1,0]+tcMatrix[1,1])]])
    return retValue
```

Look at this for all the data:

```
allDataMLEMatrix = makeMLEMatrix(allTransitionCounts)
allDataMLEMatrix
```

```
P                   # compare to made up probs in toy model
```

As we said before, we can concentrate just on two unknowns $(\hat{p}_{0,0}, \hat{p}_{1,1})$, so we can make a function just to return this tuple:

```
%auto
def makeMLE00And11(tcMatrix):
    '''Return an MLE tuple (p00, p11) from given 2-state
transition count data.

    Param tcMatrix is a 2x2 matrix of transition counts.
    Returns (n_00/(n_00+n_01, n_11/(n_10+n_11) from tcMatrix.
    Returns null if there is not at least one count in each row
of tcMatrix. '''

    retValue = None
    if (tcMatrix[0] > 0) and (tcMatrix[1] > 0):
        retValue =
(RR(tcMatrix[0,0]/(tcMatrix[0,0]+tcMatrix[0,1])),
RR(tcMatrix[1,1]/(tcMatrix[1,0]+tcMatrix[1,1])))
```

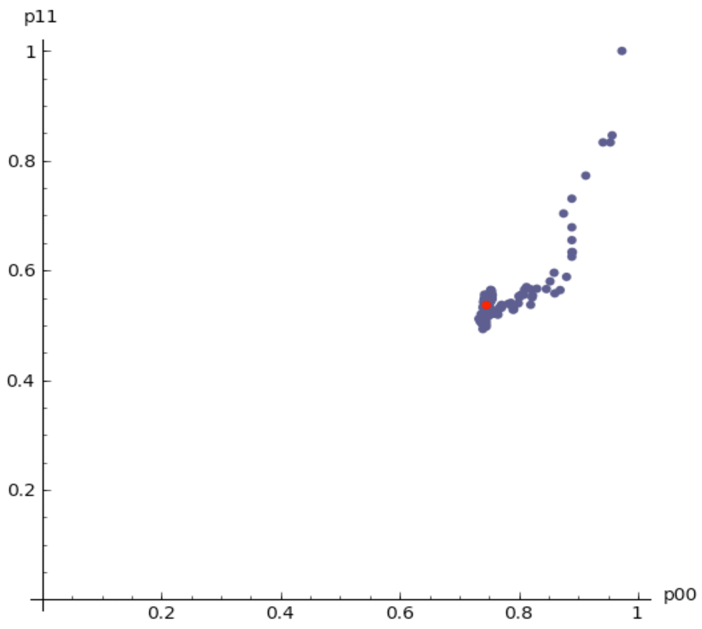
```
    return retValue
```

What is $(\hat{p}_{0,0},\hat{p}_{1,1})$ using all our data?

```
allDataMLE00And11 = makeMLE00And11(allTransitionCounts)
allDataMLE00And11
```

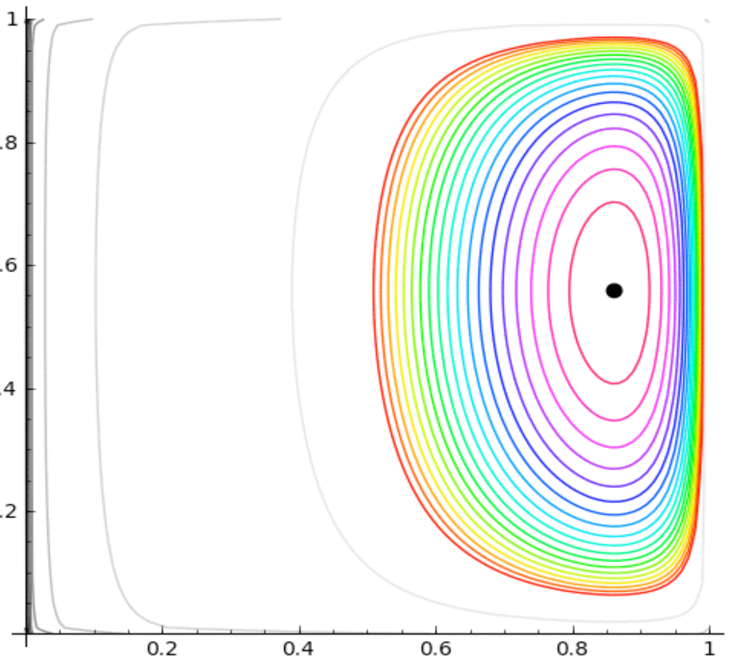
We can use our log-likelihood function in the form of a Sage symbolic function with symbolic variables `n00, n01, n10, n11, p00, p01`, and substitute in the values we have just found, using all our data, for all of these variables, to find the maximum of the log-likelihood function (i.e. the value of the function evaluated at the MLE).

Here is a plot of $(\hat{p}_{00},\hat{p}_{11})$, moving as the amount of data increases. It loops continually so if it looks like it is not moving, it is towards the end when the MLE has settled down - just wait a short while and the loop will start again:



Animation of the MLE as the amount of data increases

Here is an animated contour plot of our log-likelihood function, moving as the amount of data increases, with the MLE indicated as the black dot ●.   Again, it loops continually:



Animated contour plot of the log-likelihood function for P as data increases

```
#just the final likelihood contour plot
# use maximum of log lik to calculate come contour values for a
contour plot
# do this by evaluating L with all our data
maxLogL= L.subs(n00=allTransitionCounts[0,0],
n01=allTransitionCounts[0,1], n10=allTransitionCounts[1,0],
n11=allTransitionCounts[1,1], p00=allDataMLE00And11[0],
p11=allDataMLE00And11[1])
# make a list of contours
ourContours = tuple([maxLogL-2*i for i in range(0,20,1)])
# make a contour plot
cp=contour_plot(L.subs(n00=allTransitionCounts[0,0],
n01=allTransitionCounts[0,1], n10=allTransitionCounts[1,0],
n11=allTransitionCounts[1,1]), (p00, 0.0001, .9999), (p11,
.0001, .9999),fill=False, aspect_ratio=1, contours=10)
cp+=contour_plot(L.subs(n00=allTransitionCounts[0,0],
n01=allTransitionCounts[0,1], n10=allTransitionCounts[1,0],
n11=allTransitionCounts[1,1]), (p00, 0.0001, .9999), (p11,
.0001, .9999),fill=False, aspect_ratio=1,contours=ourContours,
cmap='hsv')
cp+=point(allDataMLE00And11,pointsize=50,rgbcolor='black')
cp.show()
```

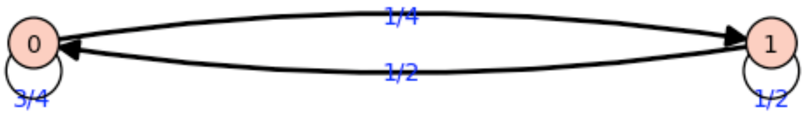
You Think: What is the MLE of θ in an product $Bernoulli(\theta)$ experiment for the problem, i.e., we now model

$$X_0, X_1, \ldots, X_n \overset{IID}{\sim} Bernoulli(\theta)$$

```
# what is the MLE thetahat of the wet or dry (1 or 0) days under
IID Bernoulli(theta) RV
makeFreqDict(x0ton)
```

Here is a nice trick to make a flow diagram fast and dirty in Sage. For our Christchurch Dry-Wet chain with MLE $\widehat{\mathbf{P}}$ we can do the following flow diagram.

```
P = matrix([[3/4,1/4],[1/2,1/2]])  # construct and assign the
matrix to P
p = DiGraph(P,format="weighted_adjacency_matrix")
pos_dict={}
pos_dict[0] = [1,1]
pos_dict[1] = [3,1]
p.plot(edge_labels=True,pos=pos_dict,vertex_size=300).show()
```



You Try: Consider the Markov chain describing the mode of transport used by a lazy professor. He has only two modes of transport, namely Walk or Drive. Label Walk by 0 and Drive by 1. If he walks today then he will definitely drive tomorrow. But, if he drives today then he flips a fair coin to decide whether he will Walk or Drive tomorrow. His decision to get to work is the same on each day. In the cells below try to:

- Find the flow diagram
- Find and assign the transition probability matrix for this Markov chain
- Find the probability that he will drive on the n-th day given he will walk today (day 0)
- What is the steady state probability vector for this chain.

```
# making the animation for the moving MLE - start by making
tuples to plot
# too much data to take every day - start with every 10 days
ns = []
MLE00And11s = []
most_is = range(1,min(20,len(all_daysdata)))
if len(all_daysdata) > 20: most_is = most_is + range(20,
len(all_daysdata),10)
most_is.append(len(all_daysdata))
for i in most_is:

    tcCounts_i = makeTransitionCounts(all_daysdata[0:i])
    # only do plot if there is at least one count in both rows
of the trans count matrix
    if (tcCounts_i[0] > 0) and (tcCounts_i[1] > 0):
        MLE00And11_i = makeMLE00And11(tcCounts_i) # get the MLE
        ns.append(i)
        MLE00And11s.append(MLE00And11_i)

p00Against_n = zip(ns, [p[0] for p in MLE00And11s])
p11Against_n = zip(ns, [p[1] for p in MLE00And11s])
```

```
# making the animation for the moving MLE - uncomment final two
lines to make animation

animDelay = 20 # delay between frames for animation
vMLE=[]
ptsize = 20
oldPtColours = (.3,.3,.5)
start = 0
endp= len(MLE00And11s)
#endp= 100
i = start
while i < endp:
    if i > start: pMLE_i = points(MLE00And11s[start:i],
pointsize = ptsize, rgbcolor=oldPtColours)
    else : pMLE_i = points((0,0), pointsize = 0)
    pMLE_i += points(MLE00And11s[i], pointsize = ptsize,
rgbcolor='red')
    vMLE.append(pMLE_i) # add a plot to the list of plots
    if i < 20: i = i + 1
    elif i < 100: i = i + 5
    elif i < 1000: i = i + 10
    elif i < 2000: i = i + 20
    else: i = i + 40

pMLE_final = points(MLE00And11s[start:endp-1], pointsize =
ptsize, rgbcolor=oldPtColours)
pMLE_final += points(MLE00And11s[endp-1], pointsize = ptsize,
rgbcolor='red')
vMLE.append(pMLE_final) # add a plot to the list of plots

#animMLEP = animate(vMLE,ymin=0,
ymax=1,xmin=0,xmax=1,aspect_ratio=1,axes_labels=('p00','p11')) #
animate
#animMLEP.gif(delay = animDelay)
```

```
# how to make the likelihood contour plot animation - uncomment
final 2 lines to do it

# too much data to do a frame for every day so try to take first
days and then up to every 10th then 100th then 500th days

v = [] # an empty list to store our animation in
animDelay = 50 # delay between frames for animation
#for i in range(1, len(all_daysdata)+1):
most_is = range(1,min(200,len(all_daysdata)),10)
if len(all_daysdata) > 200: most_is = most_is + range(200,
min(5000,len(all_daysdata)),100)
if len(all_daysdata) > 5000: most_is = most_is + range(5000,
len(all_daysdata),500)
most_is.append(len(all_daysdata))
for i in most_is:
        javascript:evaluate_cell(206,%200);
    tcCounts_i = makeTransitionCounts(all_daysdata[0:i])
    # only do plot if there is at least one count in both rows
of the trans count matrix
    if (tcCounts_i[0] > 0) and (tcCounts_i[1] > 0):
        MLE00And11_i = makeMLE00And11(tcCounts_i) # get the MLE

        maxLogL_i= L.subs(n00=tcCounts_i[0,0],
n01=tcCounts_i[0,1], n10=tcCounts_i[1,0], n11=tcCounts_i[1,1],
p00=MLE00And11_i[0], p11=MLE00And11_i[1])
        contours_i = tuple([maxLogL_i-2*i for i in
range(0,20,1)])


        cp_i=contour_plot(L.subs(n00=tcCounts_i[0,0],
n01=tcCounts_i[0,1], n10=tcCounts_i[1,0], n11=tcCounts_i[1,1]),
(p00, 0.0001, .9999), (p11, .0001, .9999),fill=False,
aspect_ratio=1, contours=10)
        cp_i+=contour_plot(L.subs(n00=tcCounts_i[0,0],
n01=tcCounts_i[0,1], n10=tcCounts_i[1,0], n11=tcCounts_i[1,1]),
(p00, 0.0001, .9999), (p11, .0001, .9999),fill=False,
aspect_ratio=1,contours=contours_i, cmap='hsv')
        cp_i+=point(MLE00And11_i, pointsize=50,
rgbcolor='black')
```

```
        v.append(cp_i) # add a plot to the list of plots
#animLikP = animate(v,aspect_ratio=1) # animate
#animLikP.gif(delay = animDelay)
```

Random Walks and Random Graphs in Sage

We get introduced to simple random walks in SAGE.

Problem:

1. Try to make simple Markov chain models as random walks on a lattice or a graph by modifying the following scripts.

```
set_random_seed(0)
v = [randint(0,1) for _ in range(10)]
v
```

```
sum(v)/float(len(v))
```

```
html('<h1>A Random Walk by William Stein</h1>')
vv = []; nn = 0
@interact
def foo(pts = checkbox(True, "Show points"),
        refresh = checkbox(False, "New random walk every time"),
        steps = (50,(10..500))):
    # We cache the walk in the global variable vv, so that
    # checking or unchecking the points checkbox doesn't change
    # the random walk.
    html("<h2>%s steps</h2>"%steps)
    global vv
    if refresh or len(vv) == 0:
        s = 0; v = [(0,0)]
        for i in range(steps):
             s += random() - 0.5
             v.append((i, s))
        vv = v
    elif len(vv) != steps:
        # Add or subtract some points
        s = vv[-1][1]; j = len(vv)
        for i in range(steps - len(vv)):
            s += random() - 0.5
            vv.append((i+j,s))
        v = vv[:steps]
    else:
        v = vv
    L = line(v, rgbcolor='#4a8de2')
    if pts: L += points(v, pointsize=10, rgbcolor='red')
    show(L, xmin=0, figsize=[8,3])
```

```
html('<h1>A 3D Random Walk</h1>') # this was done originally by
William Stein
@interact
def rwalk3d(n=(50,1000), frame=True):
    pnt = [0.,0.,0.]
    v = [copy(pnt)]
    for i in range(n):
        pnt[0] += random()-0.5
        pnt[1] += random()-0.5
        pnt[2] += random()-0.5
        v.append(copy(pnt))

show(line3d(v,color='black'),aspect_ratio=[1,1,1],frame=frame,figsize=[4,4])
```

Graph Browser, by Marshall Hampton

```
grs = ['BalancedTree', 'BullGraph', 'ChvatalGraph',
'CirculantGraph', 'CircularLadderGraph', 'ClawGraph',
'CompleteBipartiteGraph', 'CompleteGraph', 'CubeGraph',
'CycleGraph', 'DegreeSequence',
'DegreeSequenceConfigurationModel', 'DegreeSequenceExpected',
'DegreeSequenceTree', 'DesarguesGraph', 'DiamondGraph',
'DodecahedralGraph', 'DorogovtsevGoltsevMendesGraph',
'EmptyGraph', 'FlowerSnark', 'FruchtGraph', 'Grid2dGraph',
'GridGraph', 'HeawoodGraph', 'HexahedralGraph',
'HoffmanSingletonGraph', 'HouseGraph', 'HouseXGraph',
'IcosahedralGraph', 'KrackhardtKiteGraph', 'LCFGraph',
'LadderGraph', 'LollipopGraph', 'MoebiusKantorGraph',
'OctahedralGraph', 'PappusGraph', 'PathGraph', 'PetersenGraph',
'RandomBarabasiAlbert', 'RandomGNM', 'RandomGNP',
'RandomHolmeKim', 'RandomLobster', 'RandomNewmanWattsStrogatz',
'RandomRegular', 'RandomTreePowerlaw', 'StarGraph',
'TetrahedralGraph', 'ThomsenGraph', 'WheelGraph']
examples = {}
for g in grs:
    docs = eval('graphs.' + g + '.__doc__')
    for docline in docs.split('\n'):
        ex_loc = docline.find('graphs.' + g)
        if ex_loc != -1:
            end_paren_loc = docline[ex_loc:].find(')')
            ex_str = docline[ex_loc:end_paren_loc+ex_loc+1]
            ex_str = ex_str.replace('i+','2+')
            ex_str = ex_str.replace('(i','(4')
            break
    try:
        gt2 = eval(ex_str)
        examples[g] = ex_str
    except:
        grs.remove(g)
@interact
def graph_browser(graph_name = selector(grs, label = "Graph
type:"), newargs = input_box('',type=str,label='tuple of args'),
output_type = selector(['2D','3D'], default='2D')):
    base_g_str = 'graphs.' + graph_name
    docs = eval(base_g_str + '.__doc__')
    doc_ex_loc = docs.find('EXAMPLE')
    if docs.find('PLOTTING') != -1:
        doc_ex_loc = min(doc_ex_loc, docs.find('PLOTTING'))
    print docs[0:doc_ex_loc].replace('\n        ','\n')
    if newargs != '':
        try:
            t_graph = eval(base_g_str + newargs)
        except:
            print "Invalid arguments, using default"
            t_graph = eval(examples[graph_name])
    else:
        t_graph = eval(examples[graph_name])
    if output_type == '2D': show(t_graph)
    if output_type == '3D': t_graph.show3d()
```

```
%hide
%auto
def makeFreqDict(myDataList):
    '''Make a frequency mapping out of a list of data.

    Param myDataList, a list of data.
    Return a dictionary mapping each unique data value to its
frequency count.'''

    freqDict = {} # start with an empty dictionary

    for res in myDataList:

        if res in freqDict: # the data value already exists as a
key
                freqDict[res] = freqDict[res] + 1 # add 1 to the
count
        else: # the data value does not exist as a key value
            freqDict[res] = 1 # add a new key-value pair for
this new data value, frequency 1

    return freqDict # return the dictionary created

# end of makeFreqDict(...)
```