COMP 364: Computer Tools for Life Sciences

Python libraries; How to read and use an API

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Problem solving

Today's lecture will be slightly different than most

- we're going to define a problem
- then try to solve it using an unknown toolset
- this will help you to learn Python on your own

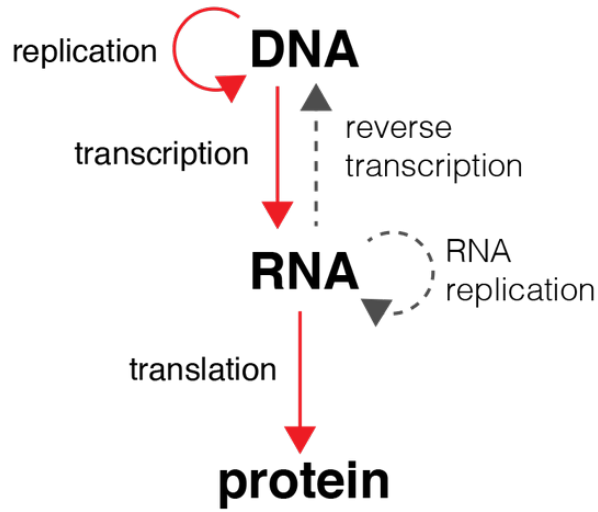
We're going to learn

- how to use Google to search for Python modules
- reading module documentation/API
  - **application programming interface (API)**

Genes and their role in a cell

Remembering the **central dogma**:

1. genes are made up of DNA
   - DNA $\in \{A, C, G, T\}$
2. genes are transcribed into RNA
   - RNA $\in \{A, C, G, U\}$
3. RNA is then translated into protein(s)



Proteins play a vital role in our survival

- the 'building blocks' of cells
- mutations in genes can lead to a malfunctioning protein
  - genes contain the instructions to build proteins
- many diseases have been linked to malfunctioning proteins
  - cystic fibrosis, Huntington's disease, etc.

Problem

To better understand the role(s) some genes play in cells

- we will group them by a **similarity measure**
- in our case, using gene expression

Gene expression can be measured by the amount of RNA found within a cell

- where each RNA is related to a gene
- the more RNA attributed to a gene, the more it was expressed

Problem:
Given a dataset containing a set of genes and their expression over a time course, group genes based on their expression between two time points.

Gene expression dataset

The gene expression dataset can be downloaded from:
`http://www.exploredata.net/Downloads/Gene-Expression-Data-Set`

This dataset includes:

- rows - 4381 observed genes
- columns - across 25 time points (in mins)
- each floating point value represents a gene's expression for a specific time point

Let's start by reading the file into memory

- and storing it in a useful data structure
  - **what would be an appropriate data structure?**

```
1  data_dict = {}
2  with open("./Spellman.csv","r") as f:
3      header = f.readline().rstrip().split(",")
4      time_points = [int(val) for val in header[1:]]
5      for line in f:
6          gene_name, *exp_counts = line.rstrip().split(",")
7          exp_counts = [float(val) for val in exp_counts]
8          try:
9              data_dict[gene_name]
10             print("Warning - multiple entries for the"
11                   "same gene '"+gene_name+"'")
12         except:
13             data_dict[gene_name] = exp_counts
14 print(len(data_dict.keys())) # prints: 4381
```

line 6 - '*' is extended iterable unpacking in Python 3

Randomly selecting dictionary keys

Okay, now let's now select 10 genes randomly to analyze

- gene names are equivalent to dictionary keys

Steps:

1. obtain a list of the dictionary's keys
2. randomly choose keys from the list

Wait, how can we figure out the Python implementation of the second step?

Randomly selecting dictionary keys #2

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Steps:

1. obtain a list of the dictionary's keys
2. randomly choose keys from the list

Wait, how can we figure out the Python implementation of the second step?

Answer: let's try Google

`http://lmgtfy.com/?q=how+to+randomly+select+keys+from+a+Python+dictionary%3F`

Randomly selecting dictionary keys #3

```
1  import random
2
3  rand_genes = random.sample(list(data_dict.keys()),k=10)
4  print(rand_genes)
5  # prints: ['YNR040W', 'YLR078C', 'YLL065W',
6  #          'YMR102C', 'YLR237W', 'YBR195C',
7  #          'YDR459C', 'YIL144W', 'YOR310C',
8  #          'YOR015W']
```

* source: https://docs.python.org/3/library/random.html

Choosing time points

Let's start by randomly selecting a pair of time points

- the early time point will be start
- the later time point will be end
- how can we do this with Python's random module?

Choosing time points #2

Let's start by randomly selecting a pair of time points

- the early time point will be start
- the later time point will be end
- how can we do this with Python's random module?

```
1  import random
2
3  start_tp = random.choice(time_points)
4  end_tp = start_tp
5  while end_tp == start_tp:
6      end_tp = random.choice(time_points)
7  print(start_tp,end_tp) # prints: 240 220
8  # ensure proper ordering of time points
9  start_tp,end_tp = sorted([start_tp,end_tp])
10 print(start_tp,end_tp) # prints: 220 240
```

Extracting expression data

Now, let's extract the gene expression data for our genes

- at the randomly chosen time points

In other words,

- For each gene that was randomly selected
- find the expression value for said gene
- at the start and end time points
- and store the expression values in a useful data structure
  - perhaps a list of tuples?
  - or can someone think of a better implementation?

```
obs = []
# obtain list indices of time points
start_index = time_points.index(start_tp)
end_index = time_points.index(end_tp)
# iterate over genes and extract expression data
for gene_name in rand_genes:
    pair = []
    pair.append(data_dict[gene_name][start_index])
    pair.append(data_dict[gene_name][end_index])
    obs.append(tuple(pair))
print(obs)
# prints:
#    [(-0.48, 0.49), (0.0, -0.05), (0.06, -0.24),
#     (0.41, -0.4), (0.09, 0.43), (0.01, 0.36),
#     (-0.06, 0.29), (-0.24, 0.53), (0.19, -0.24),
#     (0.52, -0.32)]
```

Putting it together

Okay, now that we have a list that contains

- expression data for
- 10 randomly selected genes at
- two randomly chosen time points

How can we group these genes together based on their expression?

Putting it together #2

Okay, now that we have a list that contains

- expression data for
- 10 randomly selected genes at
- two randomly chosen time points

How can we group these genes together based on their expression?

Answer: Google

`http://lmgtfy.com/?q=how+to+group+genes+expression`

Clustering

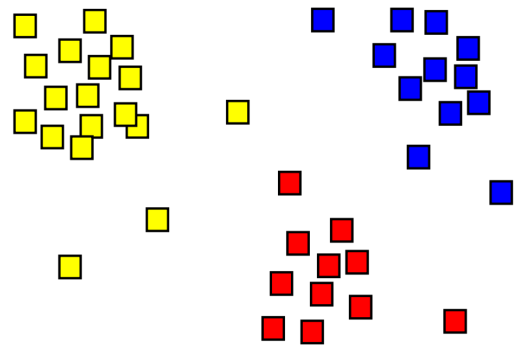
Clustering (or sometimes called 'cluster analysis')

- is the task of grouping a set of objects
- in such a way that objects in the same group (**cluster**)
- are more similar to each other than to those in other groups

How can we possibly learn to cluster gene expression data in Python?

Answer: Google! (hmmm.... a trend is forming here)

`http://lmgtfy.com/?q=python+clustering+genes+expression`



SciPy clustering

SciPy pronounced ('Sigh Pie') is a popular Python module

- provides many user-friendly and efficient functions
- useful for mathematics, science and engineering

API may be accessed from:
`https://docs.scipy.org/doc/scipy/reference/`

Let's navigate the API documentation

- to find possible clustering algorithms
- and implement one clustering algorithm in our Python script

SciPy clustering #2

```
1  from scipy.cluster.vq import kmeans
2
3  k = 3
4  code_book, distortion = kmeans(obs,3)
5  print(code_book,distortion)
6  # prints:
7  #[[ 0.55333333  0.16333333]
8  # [-0.77       -0.19      ]
9  # [ 0.03166667  0.095     ]] 0.157753028754
```

Well, that's not entirely helpful

- **kmeans()** returns a list of centroid coordinates
  - a **centroid** is the centre of a cluster
- and some measure called 'distortion'

SciPy clustering #2

What's this **kmeans2()**?

```
1  from scipy.cluster.vq import kmeans2
2
3  k = 3
4  centroid,label = kmeans2(obs,3)
5  print(centroid, label)
6  # prints:
7  # [[-0.23          0.388     ]
8  # [ 0.105       -0.485     ]
9  # [ 0.05        -0.12666667]] [0 2 0 2 1 0 2 0 0 1]
```

That's better

- now we have centroid coordinates
- and a list of group/cluster labels

Next week - Matplotlib