ECS253 - Homework 2

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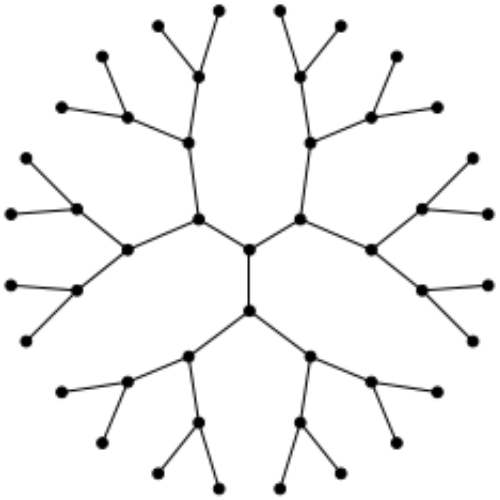
This is the common problem set for Homework 2 from the spring quarter Network Theory class at UC Davis taught by Prof. Raissa D'Souza. The original assignment is at http://mae.engr.ucdavis.edu/dsouza/Classes/253-S16/hw2.pdf. Source code for this notebook is on github at https://github.com/camillescott/ucd-ecs253.

```
In [1]: %pylab inline
        %config InlineBackend.figure_format='retina'
        import numpy as np
        import networkx as nx
        import seaborn as sns
        sns.set_style('ticks')
        sns.set_context('poster')
```

```
Populating the interactive namespace from numpy and matplotlib
```

1 The Cayley Tree

A Cayley tree is a symmetric regular tree emanating from a central node of degree k. Every node in the network has degree k, until we reach the nodes at the maximum depth d that have degree one and are called the leaves of the network. The figure below shows a Cayley tree with $k = 3$ with depth $d = 4$.



For a Cayley degree of degree k and depth d calculate:

1.1 Vertices at Exactly Distance 1

Let's start by considering a Cayley Tree at $d = 1$ (which is actually just the star graph). The central vertex, in order to have degree k, must have exactly k nodes attached directly to it. So, there are k vertices at distance 1 in this tree. If we grow the tree to higher d, the central node can have no more vertices attached, as it's already at degree k; we can then conclude, somewhat obviously, that there are k vertices at exactly distance 1.

1.2 Vertices at Exactly Distance 2

Let's consider growing the tree to $d = 2$. Each of the nodes at distance 1 already has degree 1, and so needs to have $k - 1$ nodes attached in order to grow the tree to $d = 2$. As there are k of those, there must then be $k(k - 1)$ nodes at exactly distance 2.

1.3 Vertices at Exactly Distance l

The logic for the general case follows from that for distance 2: if we expand to $d = 3$ we add another $k - 1$ nodes to each leaf, giving us $k(k - 1)^2$, and so on, meaning that there are $k(k - 1)^{l-1}$ nodes at exactly distance l.

1.4 Total Number of Vertices within Distance l

$$n(l) = 1 + \sum_{m=0..l-1} k(k-1)^m$$

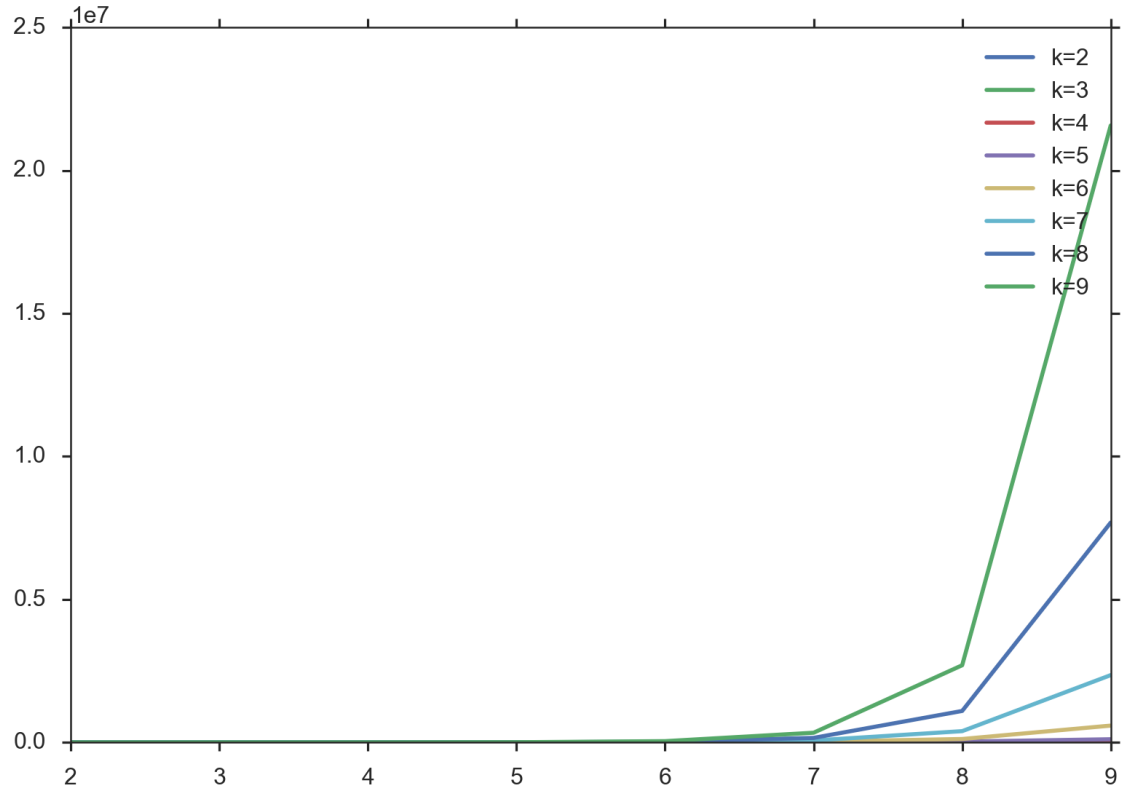
1.5 Small World

We can show the small world structure intuitively and empirically. For one, it's clear that $n(l)$ grows approximately geometrically with d and k. To illustrate this further, I've plotted $n(l)$ for increasing d with a range of k.

```
In [2]: def n_nodes_cayley(d, k):
            n = 1
            for m in range(0,d-1):
                n += k * (k-1)**m
            return n

In [3]: for k in range(2,10):
            D = range(2,10)
            plot(D, [n_nodes_cayley(d, k) for d in D], label='k={0}'.format(k))
        legend()

Out[3]: <matplotlib.legend.Legend at 0x10e2fe1d0>
```



It is also clear that the longest shortest path in this graph is always $2d$. With this and the scaling of $n(l)$, then, by approximation, we get that $d \approx log(n)/log(k)$

2 Finite size scaling

To get K_{max}, we solve the definite integral over p_k. The equation we aim to solve is then:

$$\int_1^{K_{max}} (\gamma - 1)k^{-\gamma} = N^{-1} + 1$$

.

If we expand the definite integral, we get:

$$\frac{(\gamma-1)K_{max}^{1-\gamma}}{1-\gamma} - \frac{\gamma-1}{1-\gamma} = N^{-1} + 1$$

Simplifying a bit more:

$$\frac{-K_{max}^{1-\gamma}}{1-\gamma} = N^{-1}$$

3 Analysis of a Real-world Network

I decided to attempt to build a network based on protein similarity of a group of genes. I started by downloading the FASTA-format sequence file with this query. The sequences are HOXA1 proteins in many different species.

```
In [4]: import screed
        import pandas as pd
        from networkx.drawing.nx_agraph import graphviz_layout
```

```
In [5]: !head uniprot-hox-a.fasta
```

```
>sp|P49639|HXA1_HUMAN Homeobox protein Hox-A1 OS=Homo sapiens GN=HOXA1 PE=1 SV=2
MDNARMNSFLEYPILSSGDSGTCSARAYPSDHRITTFQSCAVSANSCGGDDRFLVGRGVQ
IGSPHHHHHHHHHHPQPATYQTSGNLGVSYSHSSCGPSYGSQNFSAPYSPYALNQEADVS
GGYPQCAPAVYSGNLSSPMVQHHHHHQGYAGGAVGSPQYIHHSYGQEHQSLALATYNNSL
SPLHASHQEACRSPASETSSPAQTFDWMKVKRNPPKTGKVGEYGYLGQPNAVRTNFTTKQ
LTELEKEFHFNKYLTRARRVEIAASLQLNETQVKIWFQNRRMKQKKREKEGLLPISPATP
PGNDEKAEESSEKSSSSPCVPSPGSSTSDTLTTSH
>sp|P09022|HXA1_MOUSE Homeobox protein Hox-A1 OS=Mus musculus GN=Hoxa1 PE=1 SV=2
MNSFLEYPILGSGDSGTCSARAYPSDHGITTFQSCAVSANSCGGDDRFLVGRGVQISSPH
HHHHHHHHHHPQTATYQTSGNLGISYSHSSCGPSYGAQNFSAPYGPYGLNQEADVSGGYP
```

Pull some meta data out of the sequence headers.

```
In [6]: metadata = []
        for record in screed.open('uniprot-hox-a.fasta'):
            tokens = record.name.split()
            _, entry_ID, entry_name = tokens[0].split('|')
            kvs = tokens[-3:]
            #_, _, species = kvs[0].partition('=')
            _, _, gene_name = kvs[0].partition('=')
            _, _, evidence = kvs[1].partition('=')
            metadata.append({'blast_ID': tokens[0],
                             'entry_ID': entry_ID,
                             'entry_name': entry_name.upper(),
                             'gene_name': gene_name.upper(),
                             'evidence': evidence})
        metadata = pd.DataFrame(metadata)
        metadata.set_index('blast_ID', inplace=True)
```

We'll do the alignments with NCBI BLAST. First, make the database:

```
In [19]: !makeblastdb -dbtype prot -in uniprot-hox-a.fasta
```

```
Building a new DB, current time: 05/03/2016 11:37:15
New DB name:   uniprot-hox-a.fasta
New DB title:  uniprot-hox-a.fasta
Sequence type: Protein
Keep Linkouts: T
Keep MBits: T
Maximum file size: 1000000000B
Adding sequences from FASTA; added 632 sequences in 0.0311999 seconds.
```

Now do find the alignments. We align the sequence file against itself to get all-by-all comparisons.

```
In [20]: !blastp -query uniprot-hox-a.fasta -db uniprot-hox-a.fasta -outfmt 6 -out
```

```
In [7]: def parse_blast(filename):
            results = pd.read_csv(filename, delimiter='\t',
                                  names=['qseqid', 'sseqid', 'pident', 'length',
                                         'mismatch', 'gapopen', 'qstart', 'qend',
                                         'sstart', 'send', 'evalue', 'bitscore'])
            return results
```

The alignments are easier to intrepret. To convert them into a network, we treat `qqeqid` as a node u, `sseqid` as a node v, and the alignment as an edge e. We can weight the edge by `pident`, the percent identity from the alignment.

```
In [8]: alignments = parse_blast('uniprot-hox-a.self.blastp.tab')
```

```
In [9]: alignments.head()
```

Out[9]:

	qseqid	sseqid	pident	length	mismatch	gapopen	qstart	qend	sstart	send	evalue	bitscore
0	sp|P49639|HXA1_HUMAN	sp|P49639|HXA1_HUMAN	100.00	335	0	0	1	335	1	335	0.0	695.0
1	sp|P49639|HXA1_HUMAN	tr|G3V6R3|G3V6R3_RAT	95.39	304	13	1	1	304	1	303	0.0	579.0
2	sp|P49639|HXA1_HUMAN	tr|B9EHK7|B9EHK7_MOUSE	94.75	305	15	1	1	304	1	305	0.0	579.0
3	sp|P49639|HXA1_HUMAN	tr|S7MQL1|S7MQL1_MYOBR	95.03	302	13	1	1	302	1	300	0.0	576.0
4	sp|P49639|HXA1_HUMAN	tr|L8I3B2|L8I3B2_9CETA	93.43	335	20	1	1	335	1	333	0.0	575.0

```
In [10]: def get_graph(data, subset=None, GraphType=nx.MultiGraph):
             if subset is not None:
                 data = data[subset]
             G = GraphType()
             G.add_weighted_edges_from(data[['qseqid', 'sseqid', 'pident']].to_reco
             return G

In [11]: def plot_degree_dist(G):
             sns.distplot(list(nx.degree(G).values()))

In [12]: def draw_graph(G):
             meta = metadata.ix[G.nodes()]
             cmap = sns.cubehelix_palette(5, start=.5, rot=-.75, as_cmap=True)

             #pos = graphviz_layout(G, )
             pos = nx.spring_layout(G, k=0.9, scale=10.0)

             nx.draw_networkx_nodes(G, pos, cmap=cmap,  node_color=list(meta.evider
                                    vmin=meta.evidence.min(), vmax=meta.evidence.ma
             nx.draw_networkx_edges(G, pos)
```

3.1 The Full Graph

The full graph is extremely dense, due to the high level of similarity between these proteins. While having 632 nodes (one for each protein), it has 283461 edges!

```
In [13]: G_full = get_graph(alignments)

In [14]: print (len(G_full.nodes()), 'nodes and', len(G_full.edges()), 'edges')

632 nodes and 283461 edges
```

This graph is extremely connected. Curiously, it still has 2 separate components.

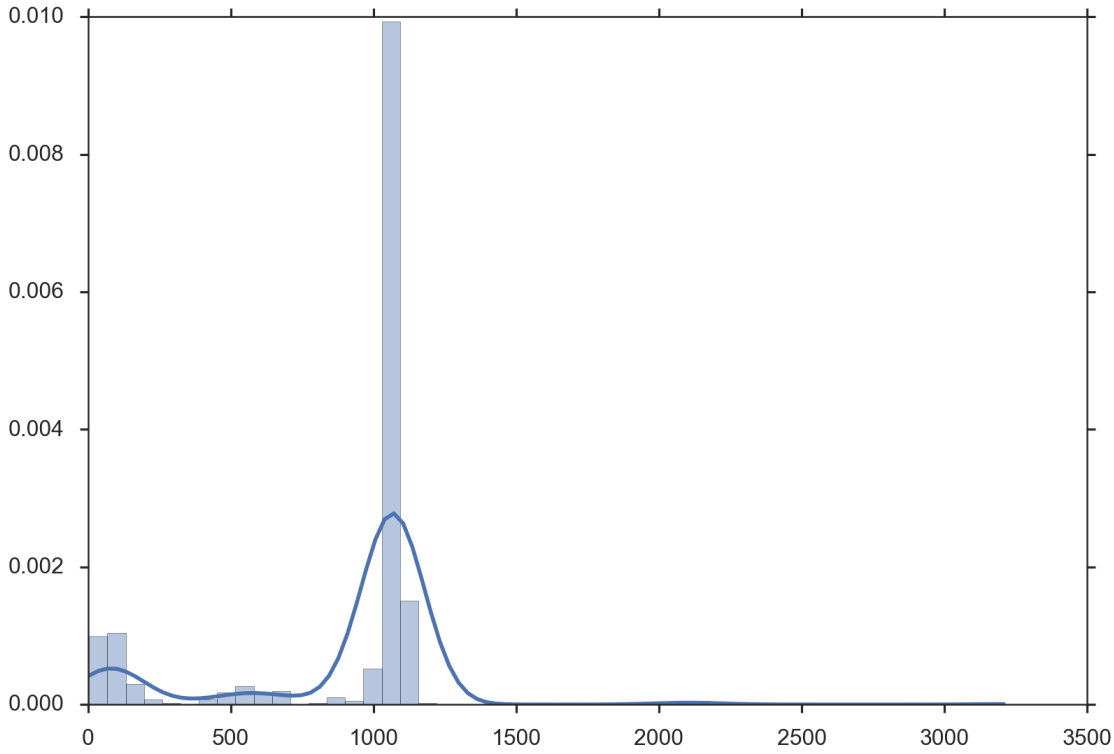
```
In [15]: nx.number_connected_components(G_full)

Out[15]: 2
```

If we look at the degree distribution, we get a bimodal distribution, which appears relatively Guassian at degree ≈ 1000.

```
In [16]: sns.distplot(list(nx.degree(G_full).values()))

Out[16]: <matplotlib.axes._subplots.AxesSubplot at 0x110eaf5c0>
```

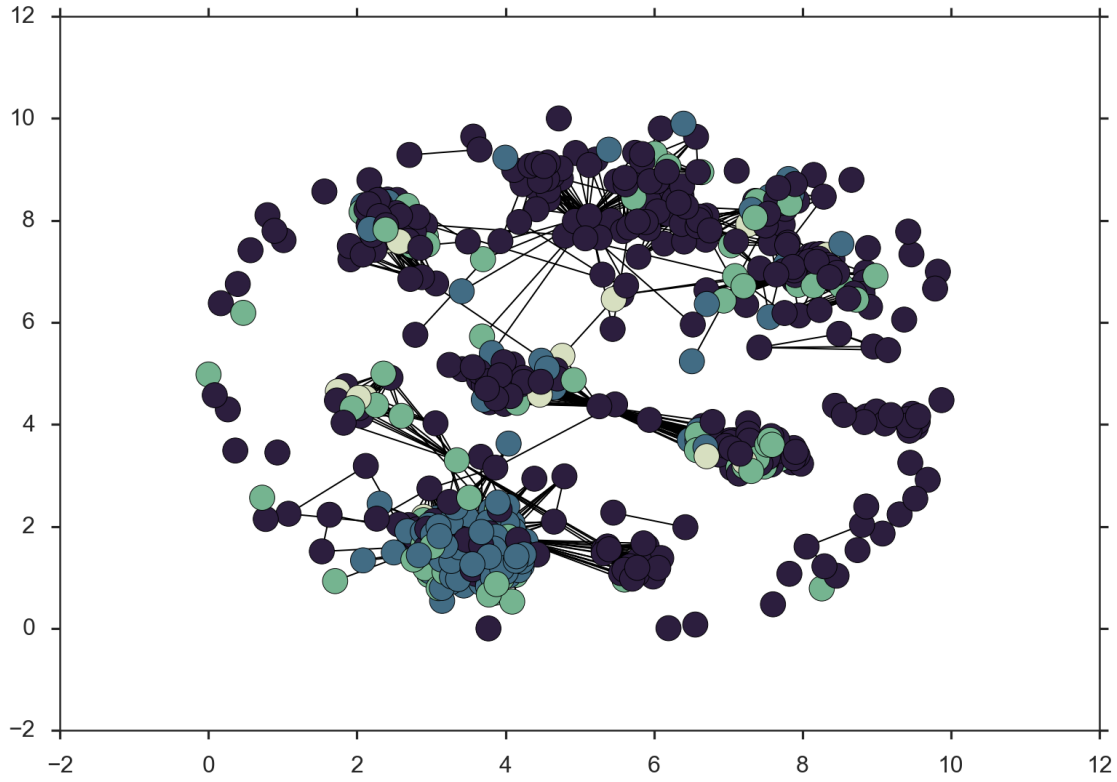


Drawing this graph would yield an incomprehensible hairball; it just has too many edges. We need to reduce its complexity.

3.2 Subselecting Good Alignments

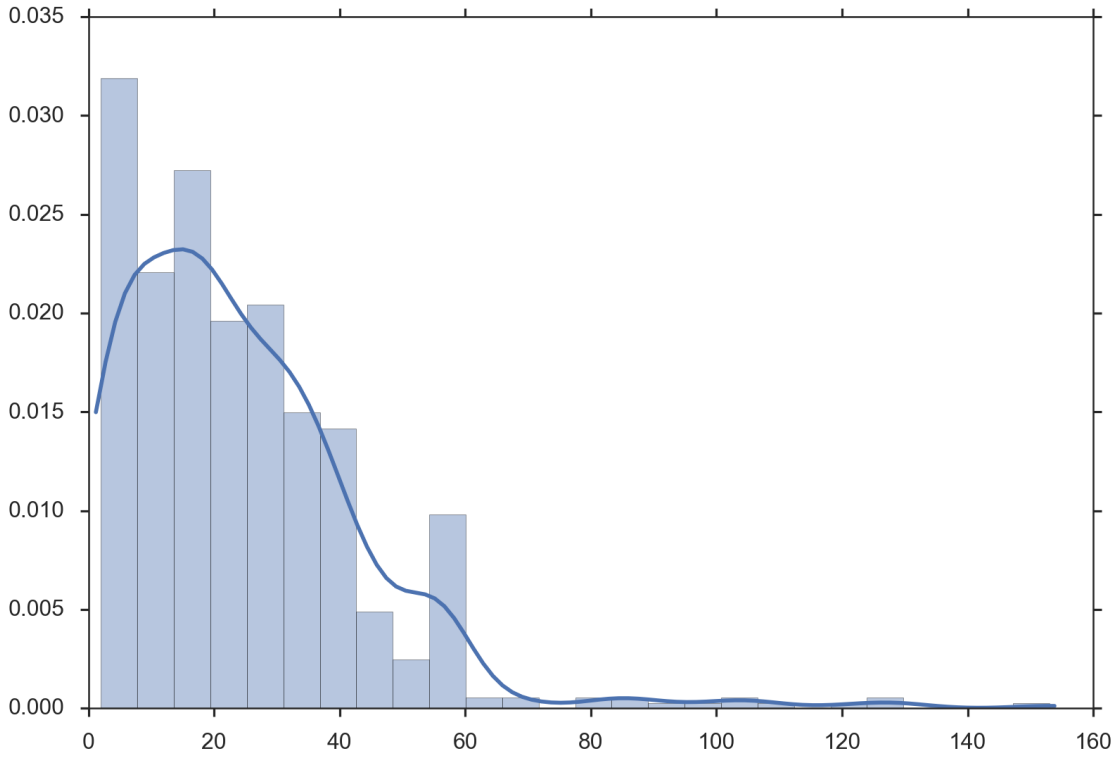
We need to prune alignments. We can easily remove aligments below a a threshold `pident` to simplify things.

```
In [21]: pident90 = get_graph(alignments, alignments.pident > 90, GraphType=nx.Grap
         draw_graph(pident90)
```



I've colored the nodes based on their *evidence* – this is a value that Uniprot assigns based on the quality of the evidence for the protein. Bad proteins are colored dark (they likely came from gene predictors), while good proteins (which likely were experimentally confirmed) are the lightest. There is some interesting structure here, namely that proteins of the same evidence tend to group. This is unsurprisingly – they probably came from the same experiment. Further, if we look at the degree distribution, it shows signs of preferential attachment; this is also unsurprising, as

```
In [22]: plot_degree_dist(pident90)
```



In [23]:
```
import community
```

In [61]:
```
def draw_communities(G):
    meta = metadata.ix[G.nodes()]
    cmap = sns.cubehelix_palette(5, start=.5, rot=-.75, as_cmap=True, reve
    N = len(G.nodes())

    partition = community.best_partition(G)
    pos = nx.spring_layout(G, k=0.9, scale=10.0)

    size = float(len(set(partition.values())))
    max_rel_size = max([len([nodes for nodes in partition.keys() if partit
                            for com in set(partition.values())])
    print (max_rel_size)
    for com in set(partition.values()) :
        list_nodes = [nodes for nodes in partition.keys() if partition[noc
        rel_size = len(list_nodes) / N
        color = [rel_size] * len(list_nodes)
        nx.draw_networkx_nodes(G, pos, list_nodes, node_color=color, cmap=
                               vmax=max_rel_size, vmin=0)

    nx.draw_networkx_edges(G, pos)
```

In [62]:
```
draw_communities(pident90)
```

```
0.1661392405063291
```