24-Networks-III-Clustering

December 6, 2016

1 Clustering and Partitioning Nodes in Graphs

Today we'll return to the subject of clustering, but now we'll be looking at nodes of a graph. Why might we want to cluster graph nodes?

- If graph nodes are our "data objects", then we might want to cluster them for all of the same reasons as we did for the case when data objects were simple records or tuples.
- Even for simple records, a distance matrix can be interpreted as a weighted graph.
- In social networks, we may want to identify communities.
- In the Web, we may want to find groups of related pages.

Outline:

1. k-core decomposition
2. Min s-t cut
3. Min cut
4. Spectral graph partitioning

1.1 K-core Decomposition

The idea behind k-core decomposition is to find a subset of a graph that represents its "core."

These are considered to be well-connected nodes that form a subgraph.

The subgraph may or may not be connected, but usually it is.

To capture this ideal formally, we say that the **k-core** of $G = (V, E)$ is a **subgraph** G_k of G such that all nodes in G_k have degree at least k.

The code number of a node n is $c(n)$ if n is contained in the $c(n)$ core but not in the $c(n) + 1$ core.

The set of all k-cores of a graph is its **k-core decomposition.**

In practice, there is a simple, intuitive way to compute the k core decomposition of a graph.

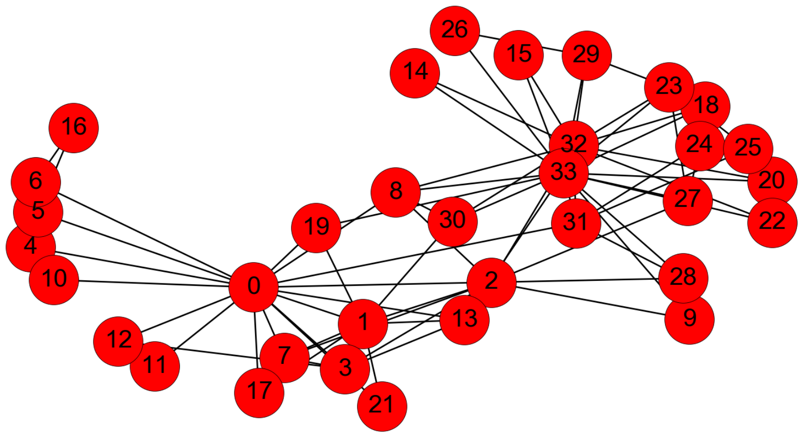
Start with a graph G whose maximum degree is m.

```
   for n in range(1,m):  remove all nodes of degree n repeat above step
until node nodes of degree n are left all nodes removed form the n-core
```

```
In [4]: G=nx.karate_club_graph()
        G = nx.Graph(G)
        np.random.seed(2)
        pos = nx.spring_layout(G)
        print('G has {} nodes and maximum degree {}'.format(len(G), max(nx.degree(G
```

```
G has 34 nodes and maximum degree 17
```

```
In [5]: fig = plt.figure(figsize=(12,6))
        ax = plt.subplot(111)
        nx.draw(G, pos=pos, with_labels=True, node_size=1000, font_size=16, ax=ax)
```

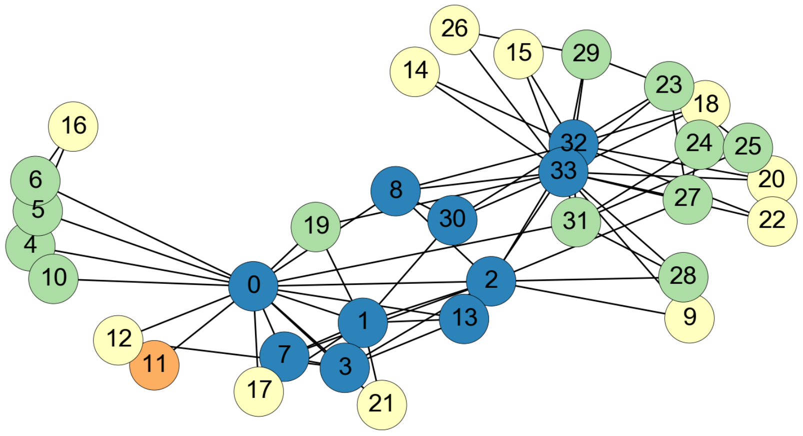


Let's compute its k-core decomposition.

```
In [6]: core_dec = nx.core_number(G)
```

Nodes with the same color are in the same k-shell:

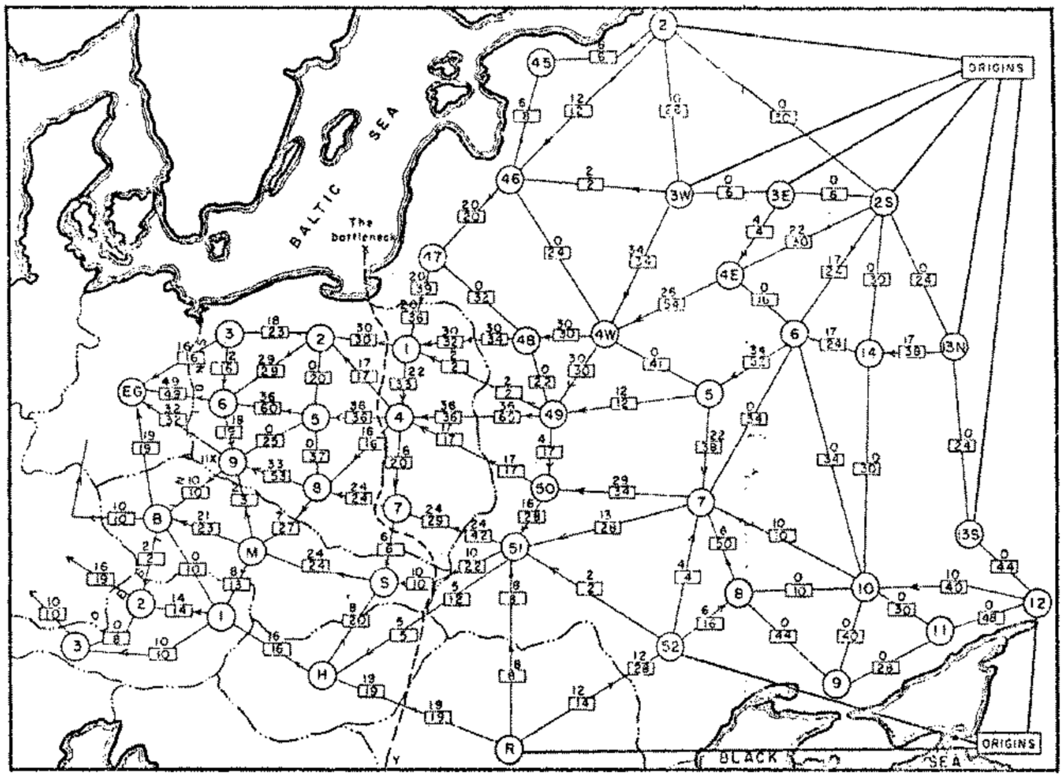
```
In [7]: fig = plt.figure(figsize=(12,6))
        ax = plt.subplot(111)
        colors = ['#d7191c', '#fdae61', '#ffffbf', '#abdda4', '#2b83ba']
        node_colors = [ colors[core_dec[v]] for v in G.nodes()]
        nx.draw(G, pos = pos, node_color=node_colors, with_labels=True, node_size=1
```



1.2 Min s-t cut

Let us say we have a graph G and two nodes in mind, s and t.

We would like to isolate s from t. What is the cheapest way to do it?



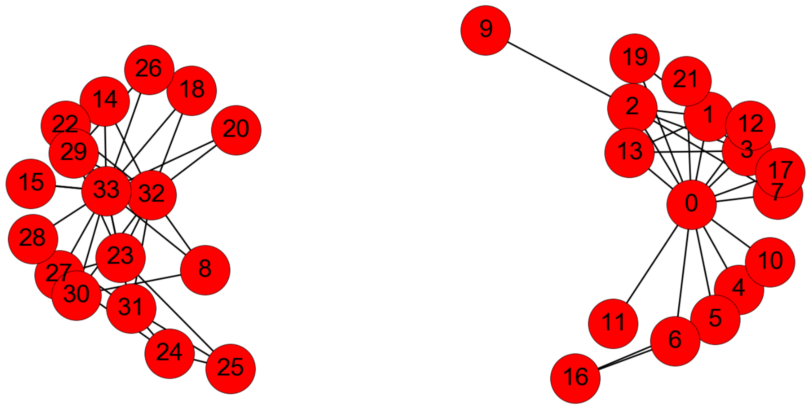
A min s-t cut problem is as follows.
We are given a weighted graph $G = (V, E)$.
An s-t cut C of G is a partition of V into $(U, V - U)$ such that $s \in U$ and $t \in V - U$.
The **cost** of a cut is the total weight of the edges that go between the two parts:

$$\text{Cost}(C) = \sum_{e(u,v), u \in U, v \in V-U} w(e)$$

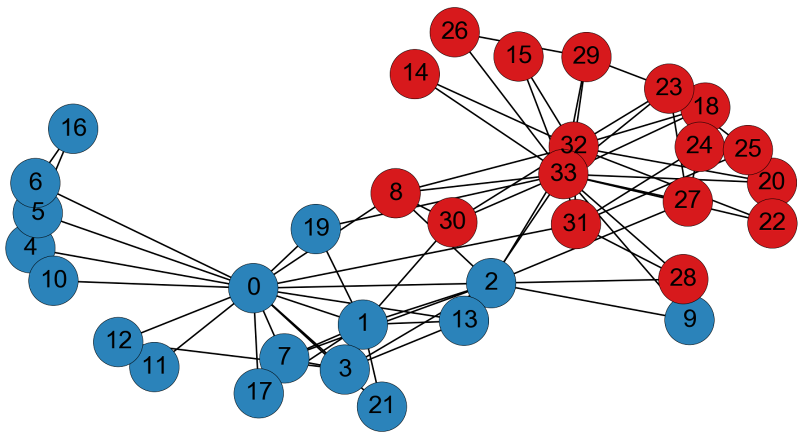
This is a very famous problem that can be solved in time that is polynomial in $|V|$ and $|E|$.
Increasingly better solutions have been found over the past 60+ years.
Looking at the karate club, the two key members are numbers 0 and 33. Let's look at that s-t cut:

```
In [9]: cut_edges = nx.minimum_edge_cut(G, s=0, t=33)
        cut_edges

Out[9]: {(0, 8),
         (0, 31),
         (1, 30),
         (2, 8),
         (2, 27),
         (2, 28),
         (2, 32),
         (9, 33),
         (13, 33),
         (19, 33)}
```

```
In [10]: Gcopy = G.copy()
         Gcopy.remove_edges_from(cut_edges)
         fig = plt.figure(figsize=(12,6))
         ax = plt.subplot(111)
         nx.draw(Gcopy, with_labels='True', node_size=1000, font_size=16, ax=ax)
```



```
In [11]: cc = nx.connected_components(Gcopy)
         node_set = {node: i for i, s in enumerate(cc) for node in s}
         colors = ['#d7191c', '#2b83ba']
         node_colors = [ colors[node_set[v]-1] for v in G.nodes()]
         fig = plt.figure(figsize=(12,6))
         ax = plt.subplot(111)
         nx.draw(G, node_color=node_colors, pos=pos, with_labels='True', node_size=
```

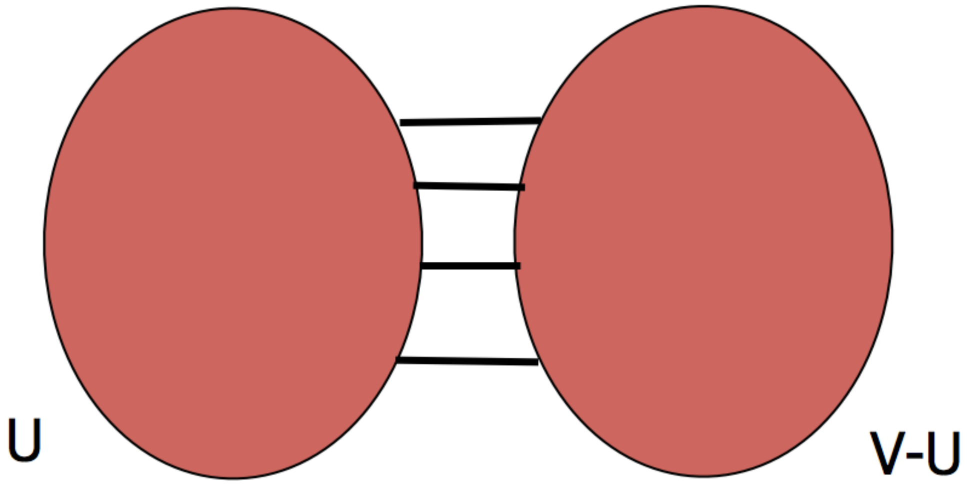


In fact, when Wayne Zachary studied the club, a conflict arose between the instructor and the president (nodes 0 and 33).

Zachary predicted the way the club would split based on an s-t min cut.
In fact, he predicted every single member's eventual association accurately except for node 8!

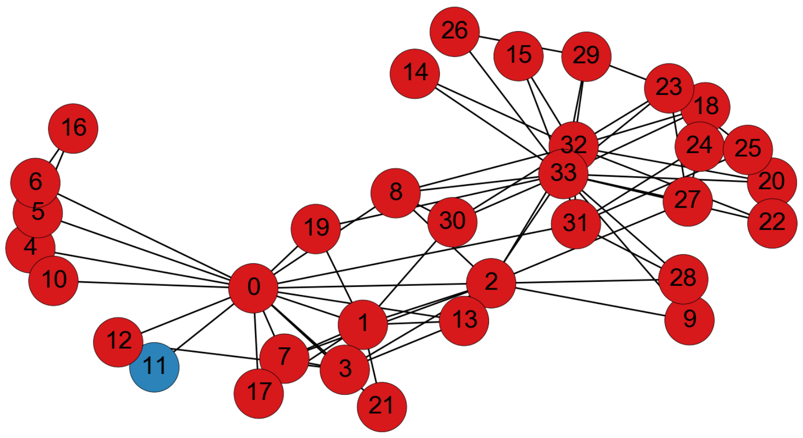
1.3 Minimum Cuts

Now, in partitioning a graph, we may not have any particular s and t in mind.
Rather, we may want to simply find the "cheapest" way to disconnect the graph.
Clearly, we can do this using s-t min cut, by simply trying all s and t pairs.



```
In [13]: Gcopy = G.copy()
         Gcopy.remove_edges_from(nx.minimum_edge_cut(G))
         cc = nx.connected_components(Gcopy)
         node_set = {node: i for i, s in enumerate(cc) for node in s}
```

```
In [14]: colors = ['#d7191c', '#2b83ba']
         node_colors = [colors[node_set[v]] for v in G]
         fig = plt.figure(figsize=(12,6))
         ax = plt.subplot(111)
         nx.draw(G, node_color=node_colors, pos=pos, with_labels='True', node_size=
```



This is in fact the minimum cut: node 11 only has one edge to the rest of the graph, so the min cut is 1.

However this is not a good approach for clustering or partitioning in general – we need to adjust our definition.

Isoperimetric Number.

The idea to avoid the problem above is to normalize the cut by the size of the smaller of the two components.

The problem above would be avoided because the smaller of the two cuts is just a single node.

This leads us to define the **isoperimetric ratio**:

$$\alpha = \frac{E(U, V \setminus U)}{\min(|U|, |V \setminus U|)}$$

And the **isoperimetric number of G:**

$$\alpha(G) = \min_U \frac{E(U, V \setminus U)}{\min(|U|, |V \setminus U|)}$$

The idea is that finding $\alpha(G)$ gives a *balanced cut* – one that maximizes the number of disconnected nodes per edge removed.

How easily can we compute this?

Unfortunately, it's not computable in polynomial time.

However, we can make good approximations, which we'll look at now.

For every $U \subset V$, $\alpha(G) \geq \lambda_2(1 - s)$ where $s = |U|/|V|$.

1.4 Graph spectral analysis

To study approximations to balanced cuts, we introduce some terms.

For a graph G with adjacency matrix A, we define the graph **Laplacian** as:

$$L = D - A$$

where D is a diagonal matrix with node degrees on the diagonal.
I.e., $D = \text{diag}(d_1, d_2, d_3, \dots)$ where d_i is the degree of node i.
The Laplacian L is symmetric and positive semi-definite.
All eigenvalues of L are real and nonnegative.
L has a single eigenvalue of value $\lambda_1 = 0$. The corresponding eigenvector is $w_1 = (1, 1, 1, \dots)^T$.
This is easily seen:

$$L\mathbf{1} = \mathbf{0}.$$

(Row i of L consists of d_i on the diagonal, and d_i -1s in other positions.)
An important fact about the Laplacian is this:
The quadratic form

$$x^T L x$$

is exactly the same as

$$\sum_{(i,j)\in E} (x_i - x_j)^2$$

The second-smallest eigenvalue of L is λ_2, called the **Fiedler value.**
We know that all of the other eigenvectors of L are orthogonal to $\mathbf{1}$, because L is symmetric.
Now, another definition of the second smallest eigenvalue is:

$$\lambda_2 = \min_{\|x\|=1, x\perp\mathbf{1}} x^T L x$$

Note that another way of saying that $x \perp \mathbf{1}$ is that the entries of x sum to 0.
The corresponding eigenvector is called the **Fiedler vector.**
It minimizes:

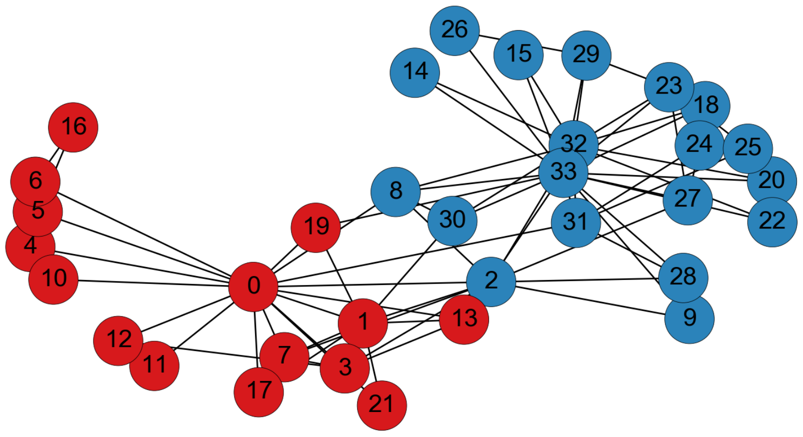
$$w_2 = \arg \min_{\|x\|=1, x\perp\mathbf{1}} \sum_{(i,j)\in E} (x_i - x_j)^2$$

Let's look at this closely:
if we think of x_i as a "coordinate" for node i in the graph,
then choosing $x = w_2$ (the eigenvector of λ_2) puts each node in a position that minimizes the sum of the "stretching" of each edge.
This is exactly the "spring" layout that we previously discussed, but in only one dimension.
Recall that the spring layout was time consuming to compute in multiple dimensions, but it turns out to have this elegant, closed form in one dimension.
So w_2 will group strongly-connected nodes together.
This leads to key ideas in node paritioning.
The basic idea is to partition nodes according to the Fiedler vector (w_2).
This can be shown to have provably good performance for the **balanced cut** problem.
There are a number of options for how to split based on the Fiedler vector.
If w_2 is the Fiedler vector, then split nodes according to a value s:

- bisection: s is the median value in w_2
- ratio cut: s is the value that maximizes α
- sign: separate positive and negative vaues ($s = 0$)
- gap: separate according to the largest gap in the values of w_2

1.4.1 Spectral Partitioning of the Karate-club Graph

```
In [15]: G=nx.karate_club_graph()
         G = nx.Graph(G)

In [16]: f = nx.fiedler_vector(G)
         f

Out[16]: array([-0.11213743, -0.04128789,  0.02321895, -0.05549978, -0.28460452,
                -0.32372722, -0.32372722, -0.052586  ,  0.05160127,  0.09280087,
                -0.28460452, -0.21099295, -0.10946129, -0.01474197,  0.16275078,
                 0.16275078, -0.42276533, -0.10018142,  0.16275078, -0.01363713,
                 0.16275078, -0.10018142,  0.16275078,  0.15569457,  0.15302558,
                 0.16096292,  0.18710959,  0.12766405,  0.0951523 ,  0.16765033,
                 0.07349963,  0.09875343,  0.13034546,  0.11890326])

In [17]: s = np.zeros(len(f),dtype='int')
         s[f>0]=1
         print(s, type(s))

[0 0 1 0 0 0 0 0 1 1 0 0 0 0 1 1 0 0 1 0 1 0 1 1 1 1 1 1 1 1 1 1 1 1] <class 'numpy


In [18]: fig = plt.figure(figsize=(12,6))
         ax = plt.subplot(111)
         colors = ['#d7191c', '#2b83ba']
         node_colors = [colors[s[v]] for v in G]
         nx.draw(G, pos=pos, node_color=node_colors, with_labels='True',node_size=1
```



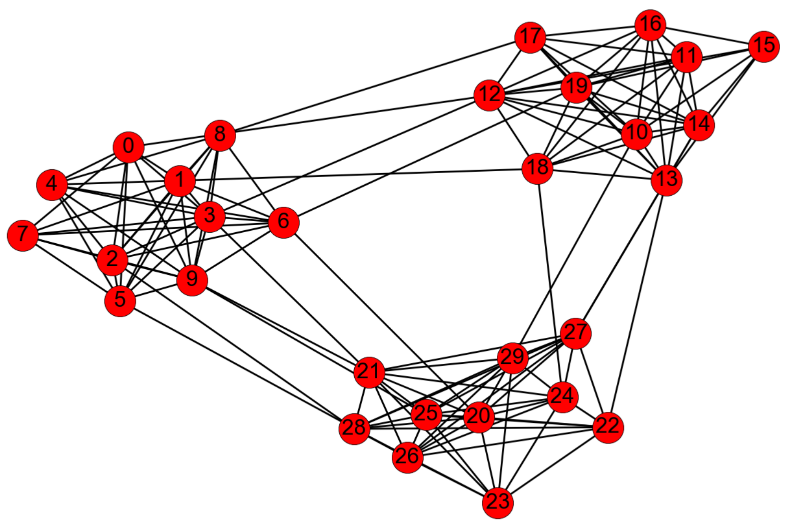
Interestingly, this is almost the same as the s-t min cut based on the president and instructor!

1.4.2 Exploring a union of noisy cliques

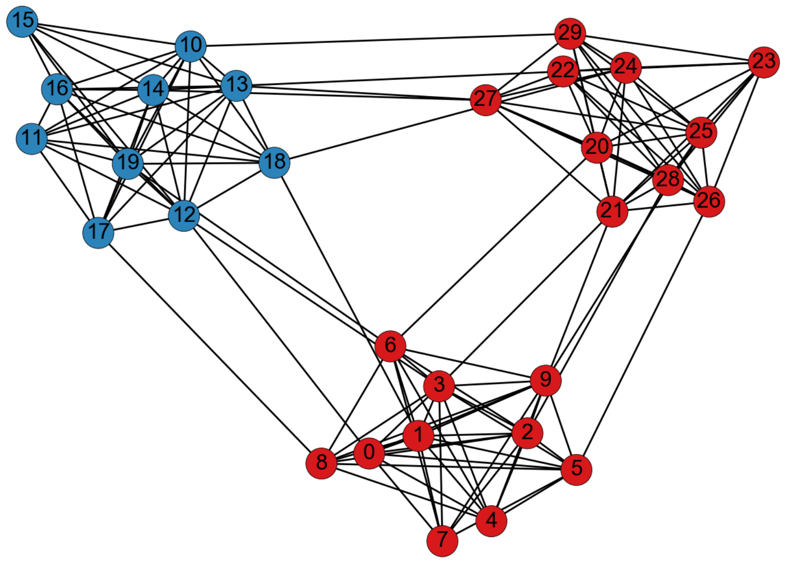
```
In [19]: from numpy.random import RandomState

         def generate_noisy_subcliques(nodes_per_clique, inside_p, across_p, min_nc
             """Generates a graph which consists of small cliques connected with ea
             The noise within a clique and across cliques can be set by the `inside
             `across_p` parameters respectively.   This is also called a "stochasti


             Parameters
             ----------
             nodes_per_clique : list
                 The size of this list corresponds to the number of cliques that wi
                 generated. The value of each element will be the size of the corre
                 clique.

             inside_p : float
                 The probability of an edge inside a clique. The higher this numbe
                 each clique will resemble a fully connected graph.

             across_p : float
                 The probability of an edge across cliques.

             min_node_label : int, default is 0
                 The minimum node label of the graph.

             seed : int, default is None
                 The seed to the pseudorandom number generator.


             Returns
             -------
             G : networkX graph
                 The generated graph.
             """

             prng = RandomState(seed)
             clique_list = []
             number_of_cliques = len(nodes_per_clique)

             # Make the independent cliques
             starting_node = min_node_label
             for clique in range(number_of_cliques):
                 G = nx.Graph()
                 for u in range(starting_node, starting_node + nodes_per_clique[cli
                     for v in range(u + 1, starting_node + nodes_per_clique[clique]
                         if prng.rand() < inside_p:
```

```
                    G.add_edge(u, v)
            clique_list.append(G)
            starting_node += nodes_per_clique[clique]

        # Combine them in one graph
        G = nx.Graph()
        for clique in range(number_of_cliques):
            G.add_edges_from(clique_list[clique].edges())

        # Connect edges across the cliques
        for i in range(number_of_cliques):
            clique_from = clique_list[i]
            for j in range(i + 1, number_of_cliques):
                clique_to = clique_list[j]
                for u in clique_from.nodes():
                    for v in clique_to.nodes():
                        if prng.rand() < across_p:
                            G.add_edge(u, v)
        return G
```

```
In [20]: nodes_per_clique = [10, 10, 10]
         across_p = 0.05
         inside_p = 0.9
         cliques = generate_noisy_subcliques(nodes_per_clique, inside_p, across_p)
         nx.draw(cliques, with_labels=True)
```



```
In [21]: f = nx.fiedler_vector(cliques)
         f

Out[21]: array([-0.13135684, -0.12976885, -0.16423764, -0.12901977, -0.16687844,
                -0.16892816, -0.11894606, -0.17545151, -0.11786813, -0.16075961,
                 0.25267838,  0.28833207,  0.21274952,  0.22492978,  0.25654525,
                 0.31537155,  0.29143408,  0.24684475,  0.20228022,  0.24919989,
                -0.12309603, -0.13221044, -0.08227062, -0.1334207 , -0.08514903,
                -0.12739927, -0.12823993, -0.04757286, -0.13264527, -0.08514633])

In [22]: s = np.zeros(len(f),dtype='int')
         s[f>0]=1
         print(s, type(s))

[0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0] <class 'numpy.ndarray


In [23]: colors = ['#d7191c', '#2b83ba']
         node_colors = [colors[s[v]] for v in cliques.nodes()]
         nx.draw(cliques, node_color=node_colors, with_labels='True')
```



1.5 Spectral Clustering

In many cases we would like to move beyond graph partitioning, to allow for clustering into k clusters.

The idea of spectral clustering takes the observations about the Fiedler vector and extends them to more than one dimension.

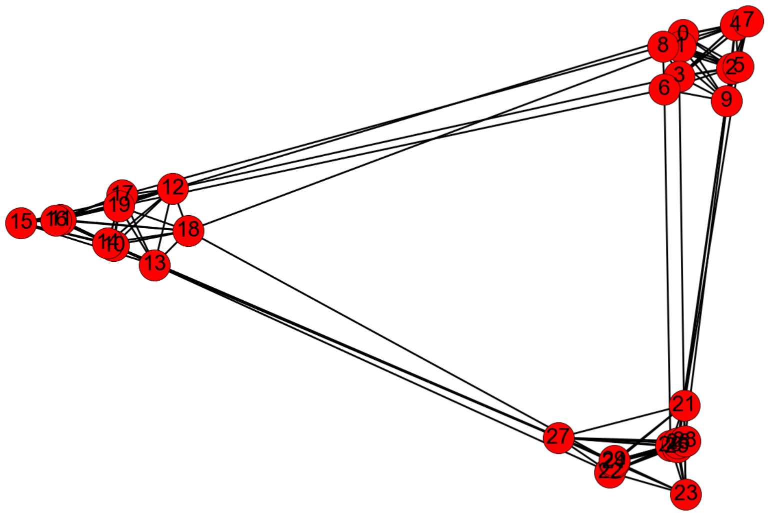
The basic idea is: * use enough of the smallest eigenvectors to properly "spread out" the nodes * cluster the nodes in the space created by this embedding.

More specifically: Given a graph G:

- Compute L, the Laplacian of G
- Compute the smallest k eigenvectors of L, excluding the smallest (the ones vector)
- Let $U \in R^{n\times k}$ be the matrix containing the eigenvectors $w_2, w_3, \ldots, w_{k+1}$ as columns
- Let the position of each node i be the point in R^k given by row i of U
- Cluster the points into k clusters using k-means

```
In [24]: L = nx.laplacian_matrix(cliques).todense()
         w, v = np.linalg.eig(L)
         v = np.array(v)
         worder = np.argsort(w)
         pos = {i: np.array([f[0], f[1]]) for i, f in enumerate(zip(v[:,worder[1]],
```

```
In [25]: colors = ['#d7191c', '#2b83ba']
         node_colors = [colors[s[v]] for v in cliques.nodes()]
         nx.draw(cliques, with_labels='True', pos=pos)
```



```
In [26]: print (v.shape, w.shape)
         worder = np.argsort(w)
         X = v @ np.diag(w)
         X = X[:,worder]

(30, 30) (30,)
```

```
In [27]: kmeans = KMeans(init='k-means++', n_clusters=3, n_init=10)
         kmeans.fit_predict(X[:,1:3])
         centroids = kmeans.cluster_centers_
         labels = kmeans.labels_
         error = kmeans.inertia_


        ---------------------------------------------------------------------------

        NameError                                 Traceback (most recent call last)

        <ipython-input-27-c07b84834d9f> in <module>()
    ----> 1 kmeans = KMeans(init='k-means++', n_clusters=3, n_init=10)
          2 kmeans.fit_predict(X[:,1:3])
          3 centroids = kmeans.cluster_centers_
          4 labels = kmeans.labels_
          5 error = kmeans.inertia_


        NameError: name 'KMeans' is not defined
```

```
In [ ]: colors = ['#d7191c', '#ffffbf', '#2b83ba', 'black']
        node_colors = [colors[labels[v]] for v in cliques]
        nx.draw(cliques, node_color=node_colors, with_labels='True', pos=pos)
```

Let's perform spectral clustering on the karate club:

```
In [ ]: k = 2
        G = nx.karate_club_graph()
        G = nx.Graph(G)
        L = nx.laplacian_matrix(G).todense()
        w, v = np.linalg.eig(L)
        worder = np.argsort(w)
        v = np.array(v)
        X = v @ np.diag(w)
        X = X[:,worder]
        kmeans = KMeans(init='k-means++', n_clusters=k, n_init=10)
```

```
kmeans.fit_predict(X[:,:k])
centroids = kmeans.cluster_centers_
labels = kmeans.labels_
error = kmeans.inertia_
colors = ['#d7191c', '#ffffbf', '#2b83ba', 'black', 'green']
node_colors = [colors[labels[v]] for v in G]
np.random.seed(2)
pos = nx.spring_layout(G)
# to understand these results, try plotting what kmeans 'sees'
# pos = {i: np.array([f[0], f[1]]) for i, f in enumerate(zip(v[:,worder[1]
fig = plt.figure(figsize=(12,6))
ax = plt.subplot(111)
nx.draw(G, node_color=node_colors, with_labels='True', pos=pos, node_size=
```