10 Spectral Clustering

Another perspective on clustering is that there are three main types: (1) *Bottom-Up*, (2) *Assignment-Based*, and (3) *Top-Down*. The bottom-up variety was like the hierarchical agglomerative clustering where we start with very small clusters and build bigger clusters. The assignment based clustering was like the k-center or the k-means variety were we "assign" each object to a center. Given the centers, there is no need to build or carve the clusters. The third type, top-down clustering, is what we will be discussing here. It starts from one big cluster and gradually divides the big clusters into smaller and smaller clusters.

At a high level the idea of top down clustering can be described very easily.

- Find the best cut of the data into two pieces.
- Recur on both pieces until that data should not be split anymore.

What remains is to determine the best way to split a set into two pieces. Then finding a threshold has similar options as with Hierarchical clustering.

Also we will need to discuss graphs, and perform clustering on graphs.

10.1 Graphs

A graph is an *abstract data type* that may seem very natural once you are familiar with and used to it. But if it is new, it may take a while to sink in. We will revisit them many times in the class.

A graph $G = (V, E)$ is defined by a set of vertices $V = \{v_1, v_2, \ldots, v_n\}$ and a set of edges $E = \{e_1, e_2, \ldots, e_m\}$ where each edge e_j is an unordered (or ordered in a directed graph) pair of edges: $e_j = \{v_i, v_{i'}\}$.

Two vertices v_1 and v_k are *connected* if there is a sequence of edges $\langle e_1, \ldots, e_{k-1}\rangle$ such that e_1 contains v_1, e_{k-1} contains v_k, and each consecutive edges can be ordered so $e_j = \{v_i, v_{i+1}\}$ and $e_{j+1} = \{v_{i+1}, v_{i+2}\}$ where the second element in e_j is the same as the first in e_{j+1}.

Consider an example graph portrayed three ways.

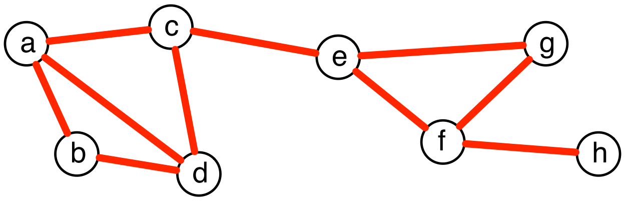
Mathematically: $G = (V, E)$ where

$$\begin{aligned} V &= \{a, b, c, d, e, f, g\} \text{ and} \\ E &= \Big\{\{a,b\}, \{a,c\}, \{a,d\}, \{b,d\}, \{c,d\}, \{c,e\}, \{e,f\}, \{e,g\}, \{f,g\}, \{f,h\}\Big\}. \end{aligned}$$

Matrix-Style: As a matrix with 1 if there is an edge, and 0 otherwise. (For a directed graph, it may not be symmetric).

$$G = \begin{array}{c|cccccccc} & a & b & c & d & e & f & g & h \\ \hline a & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ b & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ c & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ d & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ e & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ f & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ g & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ h & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{array} = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Pictorially: A ball stick model of a graph.



10.2 Clustering on Graphs

So how to cluster a graph? A cluster is a subset $S \subset V$. We are performing top down clustering, so we only need to consider a subset S and its compliment $\bar{S} = V \setminus S$.

In general, we want many edges within a cluster (small width), and few edges between clusters (large split).

- The *volume* of a cluster is $\textsf{Vol}(S) =$ the number of edges with at least one vertex in V.
- The *cut* between two clusters S, T is $\textsf{Cut}(S,T) =$ the number of edges with one vertex in S and the other in T.

Then we want a large $\textsf{Vol}(S)$ for each cluster and a small $\textsf{Cut}(S,T)$ for each pair of clusters.

Specifically, the *normalized cut* between S and T is $\textsf{NCut}(S,T) = \frac{\textsf{Cut}(S,T)}{\textsf{Vol}(S)} + \frac{\textsf{Cut}(S,T)}{\textsf{Vol}(T)}$. And we want to find the cluster S (and compliment $T = V \setminus S$) that has the *minimum* $\textsf{NCut}(S,T)$. Dividing by $\textsf{Vol}(S)$ and $\textsf{Vol}(T)$ prevents us from finding either S or T that is too small, and the $\textsf{Cut}(S,T)$ on top will force a large split.

For instance, in the above example, the minimum normalized cut is $S = \{a,b,c,d\}$, but the cluster with $S' = \{h\}$ has just as small $\textsf{Cut}(S',T')$ value. But its normalized cut is $1 + \frac{1}{10} = 1.1$, where as $\textsf{NCut}(S,T) = \frac{1}{6} + \frac{1}{5} = 0.367$.

10.2.1 Spectral Clustering

Start with an *adjacency* matrix

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

and the *degree* matrix, which along the diagonal stores the degree of each vertex. The *degree* of a vertex is the number of edges that contain that vertex.

$$D = \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Before we proceed we will want to use the matrix $D^{-1/2}$; for a diagonal matrix, a power p just takes every element $d_{i,i}$ on the diagonal to that power $d_{i,i}^p$. So

$$D^{-1/2} = \begin{pmatrix} 0.577 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.707 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.577 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.577 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.577 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.577 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.707 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then the normalized *Laplacian* matrix is now the product of $D^{-1/2}$ and A

$$I - D^{-1/2} A D^{-1/2} = \begin{pmatrix} 1 & -0.408 & -0.333 & -0.333 & 0 & 0 & 0 & 0 \\ -0.408 & 1 & 0 & -0.408 & 0 & 0 & 0 & 0 \\ -0.333 & 0 & 1 & -0.333 & -0.333 & 0 & 0 & 0 \\ -0.333 & -0.408 & -0.333 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -0.333 & 0 & 1 & -0.333 & -0.408 & 0 \\ 0 & 0 & 0 & 0 & -0.333 & 1 & -0.408 & -0.577 \\ 0 & 0 & 0 & 0 & -0.408 & -0.408 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.577 & 0 & 1 \end{pmatrix}.$$

The *eigenvector* of a matrix M is the the vector v such that

$$Mv = \lambda v,$$

where λ is a scalar. Then λ is the corresponding *eigenvalue*. We usually restrict that $\|v\| = 1$.

There are (typically) several eigenvectors of L (the normalized Laplacian): We list them here sorted by λ.

λ	0	**0.125**	0.724	1.00	1.33	1.42	1.66	1.73
V	$-.39$	0.38	$-.09$	0.00	0.71	0.26	$-.32$	0.16
	$-.32$	0.36	$-.27$	0.50	0.00	$-.51$	0.38	$-.18$
	$-.39$	0.18	0.36	$-.61$	0.00	0.03	0.47	$-.29$
	$-.39$	0.38	$-.09$	0.00	$-.71$	0.26	$-.32$	0.16
	$-.39$	$-.28$	0.48	0.00	0.00	$-.57$	0.31	0.33
	$-.39$	$-.48$	$-.29$	0.00	0.00	0.05	$-.31$	$-.65$
	$-.31$	$-.36$	0.27	0.50	0.00	0.51	0.38	$-.18$
	$-.22$	$-.32$	$-.61$	$-.35$	0.00	$-.07$	0.27	0.51

This can be calculated easily in matlab using the `[`V`,`Λ`] = eig(`L`)` command.

The first eigenvalue of the Laplacian is always 0, up to numerical error.

The second eigenvector of the normalized Laplacian is a *very important* descriptor of a graph. In the example it is $v_2 = (0.38, 0.36, 0.18, 0.38, -.28, -.48, -.36, -.32)$ as read off the second column of the above chart.

- It tells us how to best cut the graph.
- It tells us how "best" to put all of the vertices on a single line (this sometimes works better for the unnormalized Laplacian, see below. There it is called the *Fiedler vector*.)

- We can set $S = \{v_i \in V \mid u_2(v_i) < 0\}$ and $T = V \setminus S$.

  Then $S = \{a, b, c, d\}$ and $T = \{e, f, g, h\}$.

- Can sometimes do better by checking all possible cuts along v_2 (use any threshold, not only 0). Take one with best $\mathsf{NCut}(S, T)$.

The third eigenvector can be useful too. It can be used (with the second eigenvector) to lay out the vertices in $\mathbb{R}^2$, and can then be used to make a 4-way cut.

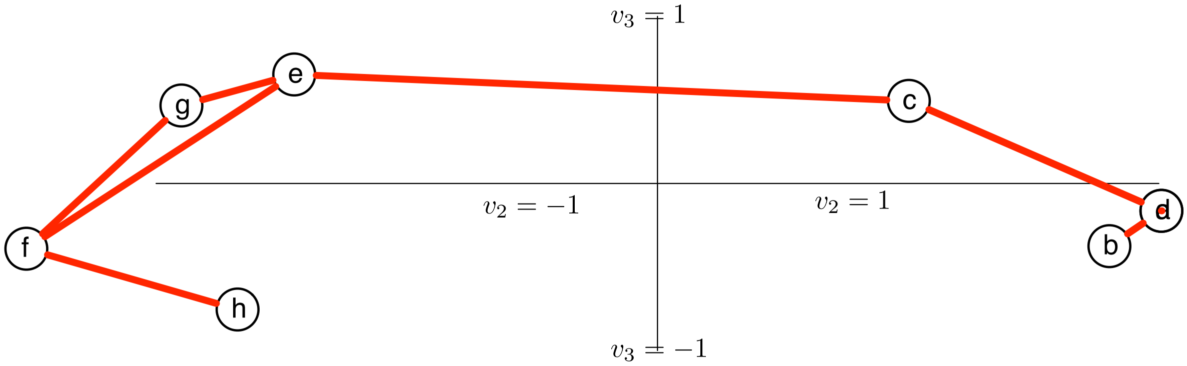
[$++$] $S = \{c\}$ defined as $v_2 > 0$ and $v_3 > 0$

[$+-$] $T = \{a, b, d\}$ defined as $v_2 > 0$ and $v_3 < 0$

[$-+$] $U = \{g, e\}$ defined as $v_2 < 0$ and $v_3 > 0$

[$--$] $R = \{f, h\}$ defined as $v_2 < 0$ and $v_3 > 0$.

When drawing the graph using v_2 and v_3 its good to scale the values by $1/\sqrt{\lambda_i}$ along each axis. Note that in the drawing below points a and d are directly on top of each other. From the perspective of the graph, they are indistinguishable. The eigenstructure does not separate them until v_5.



Alternatively, we can use the first d eigenvectors (scaled by eigenvalues) to embed the vertices in $\mathbb{R}^d$. Then we can use any Euclidean clustering algorithm (such as Lloyds for k-means clustering). The smaller the eigenvector, the more important the direction. So the larger the index of the eigenvalue, the smaller the $1/\sqrt{\lambda_i}$ will be. So the top 5 or so (depending on data) may be all required. Notice here how the second eigenvector provides much better separation than the third one.

This embedding into $\mathbb{R}^2$ is a form of *non-linear dimensionality reduction*.

Affinity matrix. More generally, the adjacency matrix need not be $0-1$. It can be filled with the *similarity* value defined by some similarity between element; then A stands for *affinity*. The diagonal is defined as the sum of elements in a row (or column — it must be symmetric). Then spectral clustering can be run as before. When the similarity of a pair is very small, it is a good heuristic to round the values down to 0 in the matrix to make the algorithm run faster.

10.2.2 (Unnormalized) Laplacian

In some contexts it will be suitable to use the (regular, unnormalized) Laplacian defined:

$$L_0 = D - A = \begin{pmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 3 & -1 & -1 & 0 & 0 & 0 \\ -1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 3 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}.$$

Note that the entries in each row and column of L_0 sum up to 0.

- think of D as the *flow* into a vertex, and
- think of A as the *flow* out of the vertex.

The water keeps flowing, so it does not get stuck anywhere. That is, as much flows in as flows out.

We can also convert L_0 to the normalized Laplacian L using the $D^{-1/2}$ matrix as

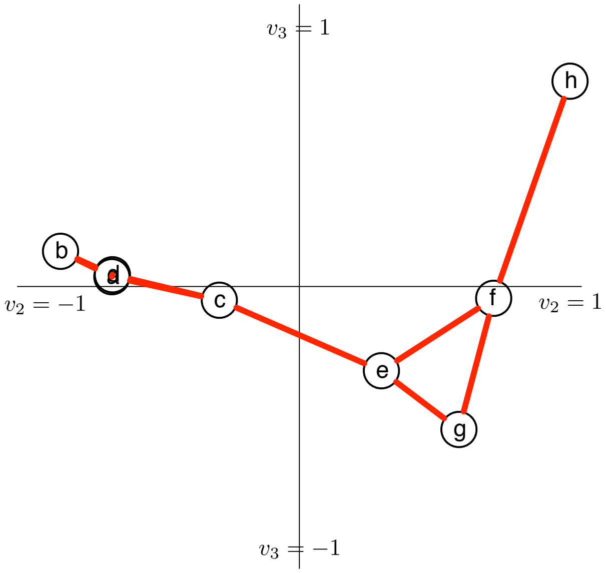
$$L = I - D^{-1/2} A D^{-1/2} = D^{-1/2} L_0 D^{-1/2}.$$

The left- and right-multiplication by $D^{-1/2}$ can be thought of as normalizing by the degrees. That is each entry $P_{i,j}$ of $P = D^{-1/2} A D^{-1/2}$ (and edge (i,j)) is normalized by the amount of flow in and out of the nodes v_i and v_j of its corresponding edge (i,j).

There are (typically) several eigenvectors of L_0 (the Laplacian). We list them here sorted by λ.

λ	0	**0.278**	1.11	2.31	3.46	4	4.82
V	$1/\sqrt{8}$	$-.36$	0.08	0.10	0.28	0.25	$1/\sqrt{2}$
	$1/\sqrt{8}$	$-.42$	0.18	0.64	$-.38$	0.25	0
	$1/\sqrt{8}$	$-.20$	$-.11$	0.61	0.03	$-.25$	0
	$1/\sqrt{8}$	$-.36$	0.08	0.10	0.28	0.25	$-1/\sqrt{2}$
	$1/\sqrt{8}$	0.17	$-.37$	0.21	$-.54$	$-.25$	0
	$1/\sqrt{8}$	0.36	$-.08$	$-.10$	$-.28$	0.75	0
	$1/\sqrt{8}$	0.31	$-.51$	$-.36$	$-.56$	0.56	0
	$1/\sqrt{8}$	0.50	0.73	0.08	0.11	0.11	0

And here is the drawing of the vertices according to v_2 and v_3, scaled by $1/\sqrt{\lambda_i}$ along each axis. Again the drawing below points a and d are directly on top of each other. From the perspective of the graph, they are indistinguishable. The eigenstructure does not separate them until v_7.


$v_3 = 1$
h
b
d
$v_2 = -1$
c
f
$v_2 = 1$
e
g
$v_3 = -1$