Clustering of Unsigned and Signed Graphs Using Normalized Graph Cuts (Normalized Cuts 15+ years later) Part II

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Special thanks to Jocelyn Quaintance, Joao Cedoc,
Jianbo Shi, and Stella Yu.

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Detailed slides in Web page for CIS515:

http://www.cis.upenn.edu/∼cis515/cis515-notes-15.html

Figure 1: Beethoven and Twitter

Review of Part I

Given a graph $G = (V, W)$ specified by a weight matrix W (with nonnegative weights), we want to *partition the set of nodes V into K clusters* by finding a partition $(A_1, \ldots, A_K)$.

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To keep the clusters reasonably balanced, we find a partition $(A_1, \ldots, A_K)$ that minimizes the *normalized cut*

$$\mathrm{Ncut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{links}(A_i, \overline{A_i})}{\mathrm{vol}(A_i)} = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_i, \overline{A_i})}{\mathrm{vol}(A_i)}.$$

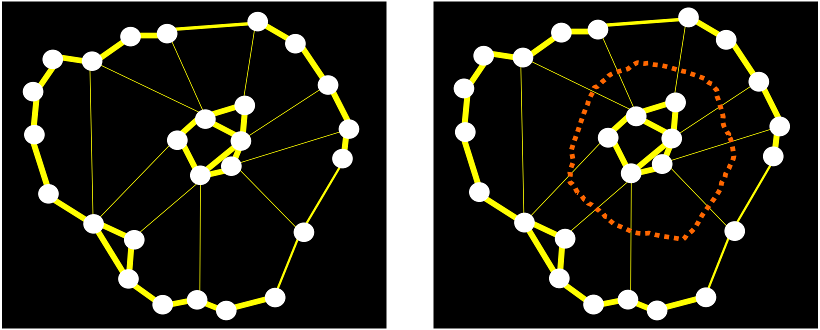

Figure 2: A weighted graph and its partition into two clusters.

We describe a partition $(A_1, \ldots, A_K)$ of the set of nodes V by an $N \times K$ matrix $X = [X^1 \cdots X^K]$ whose columns $X^1, \ldots, X^K$ are indicator vectors of the partition $(A_1, \ldots, A_K)$.

When $N = 10$ and $K = 4$, an example of a matrix X representing the partition of $V = \{v_1, v_2, \ldots, v_{10}\}$ into the four blocks

$$\{A_1, A_2, A_3, A_4\} = \{\{v_2, v_4, v_6\}, \{v_1, v_5\}, \{v_3, v_8, v_{10}\}, \{v_7, v_9\}\},$$

is shown next:

$$X = \begin{pmatrix} 0 & a_2 & 0 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_4 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_4 \\ 0 & 0 & a_3 & 0 \end{pmatrix}.$$

If we let

$$\mathcal{X} = \left\{ [X^1 \ \ldots \ X^K] \mid X^j = a_j(x^j_1, \ldots, x^j_N), \ x^j_i \in \{1, 0\}, a_j \in \mathbb{R}, \ X^j \neq 0 \right\}$$

then the problem can be stated in matrix form (using the graph Laplacian):

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then the problem can be stated in matrix form (using the graph Laplacian):

***K*-way Clustering of a graph using Normalized Cut, Version 1: Problem PNC1**

$$\begin{aligned} &\text{minimize} && \sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \\ &\text{subject to} && (X^i)^\top D X^j = 0, \quad 1 \leq i, j \leq K,\; i \neq j, \\ & && X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}, \qquad\qquad X \in \mathcal{X}. \end{aligned}$$

The solutions that we are seeking are K-tuples $(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K))$ of points in $\mathbb{RP}^{N-1}$ determined by their homogeneous coordinates $X^1, \ldots, X^K$.

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There are two possible relaxations:

Problem $(*_1)$

$$\begin{aligned} \text{minimize} \quad & \sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \\ \text{subject to} \quad & (X^i)^\top D X^j = 0, X^j \neq 0 \qquad 1 \leq i, j \leq K,\ i \neq j, \\ & X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}. \end{aligned}$$

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Problem $(*_2)$

$$\begin{aligned} &\text{minimize} && \mathrm{tr}(X^\top L X) \\ &\text{subject to} && X^\top D X = I, \\ & && X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}. \end{aligned}$$

Problem $(*_1)$

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Every solution Z of problem $(*_2)$ yields a *family of solutions* of problem $(*_1)$; namely, all matrices of the form ZQ, where Q is a $K \times K$ matrix with nonzero and pairwise orthogonal columns.

5. Finding a Discrete Solution Close to a Continuous Approximation

The next step is to find an exact solution $(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K)) \in \mathbb{P}(\mathcal{K})$ which is the closest (in a suitable sense) to our approximate solution $(Z^1, \ldots, Z^K)$.

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Since the solutions ZQ of $(*_1)$ are all equivalent (they yield the same minimum for the normalized cut), it makes sense to look for a discrete solution X closest to one of these ZQ.

If we use the Riemannian metric on $\mathbb{RP}^{N-1}$ induced by the Euclidean metric on $\mathbb{R}^N$ and the product distance on $(\mathbb{RP}^{N-1})^K$ given by

$$d\big((\mathbb{P}(X^1),\ldots,\mathbb{P}(X^K)),(\mathbb{P}(Z^1),\ldots,\mathbb{P}(Z^K))\big)=\sum_{j=1}^{K}d(\mathbb{P}(X^j),\mathbb{P}(Z^j)),$$

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it can be shown that minimizing the distance
$d\big((\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K)), (\mathbb{P}(Z^1), \ldots, \mathbb{P}(Z^K))\big)$ in $(\mathbb{RP}^{N-1})^K$
is equivalent to minimizing

$$\sum_{j=1}^{K} \left\| X^j - Z^j \right\|_2, \quad \text{subject to} \quad \left\| X^j \right\|_2 = \left\| Z^j \right\|_2 \ (j = 1, \ldots, K).$$

We are not aware of any optimization method to solve the above problem, which seems difficult to tackle due to constraints $\|X^j\|_2 = \|Z^j\|_2$ $(j = 1, \ldots, K)$.

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Therefore, we drop these constraints and attempt to minimize

$$\|X - Z\|_F^2 = \sum_{j=1}^{K} \left\|X^j - Z^j\right\|_2^2,$$

the Frobenius norm of $X - Z$. This is implicitly the choice made by Yu.

Inspired by Yu and the previous discussion, given a solution Z of problem $(*_2)$, we look for pairs (X, Q) with $X \in \mathcal{X}$ and where Q is a $K \times K$ matrix with nonzero and pairwise orthogonal columns, with $\|X\|_F = \|Z\|_F$, that minimize

$$\varphi(X, Q) = \|X - ZQ\|_F .$$

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Yu and Shi consider the special case where $Q \in \mathbf{O}(K)$.

We consider the more general case where $Q = R\Lambda$, with $R \in \mathbf{O}(K)$ and Λ is a diagonal invertible matrix.

The key to minimizing $\|X - ZQ\|_F$ rests on the following result:

$$\|X - ZQ\|_F^2 = \|X\|_F^2 - 2\mathrm{tr}(Q^\top Z^\top X) + \mathrm{tr}(Z^\top ZQQ^\top).$$

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This is a hard problem because it is a nonlinear optimization problem involving two matrix unknowns X and Q.

To simplify the problem, we proceed by *alternating steps* during which

1. we *minimize* $\varphi(X, Q) = \|X - ZQ\|_F$ *with respect to* X *holding* Q *fixed*, and
2. steps during which we *minimize* $\varphi(X, Q) = \|X - ZQ\|_F$ *with respect to* Q *holding* X *fixed*.

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This *second step in which* X *is held fixed* has been studied, but it is still a hard problem for which no closed–form solution is known. Consequently, we further simplify the problem.

Since Q is of the form $Q = R\Lambda$ where $R \in \mathbf{O}(K)$ and Λ is a diagonal invertible matrix, we minimize $\|X - ZR\Lambda\|_F$ in two stages.

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1. We set $\Lambda = I$ and find $R \in \mathbf{O}(K)$ that minimizes $\|X - ZR\|_F$.
2. Given X, Z, and R, find a diagonal invertible matrix Λ that minimizes $\|X - ZR\Lambda\|_F$.

In *stage 1*, the matrix $Q = R$ is orthogonal, so $QQ^\top = I$, and since Z and X are given, the problem reduces to minimizing $-2\mathrm{tr}(Q^\top Z^\top X)$; that is, *maximizing* $\mathrm{tr}(Q^\top Z^\top X)$.

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This is a standard result:

Proposition 1

For any two fixed $N \times K$ matrices X and Z, the minimum of the set

$$\{\|X - ZR\|_F \mid R \in \mathbf{O}(K)\}$$

is achieved by $R = UV^\top$, for any SVD decomposition $U\Sigma V^\top = Z^\top X$ of $Z^\top X$.

The following proposition takes care of *stage 2*.

Proposition 2

For any two fixed $N \times K$ matrices X and Z, where Z has no zero column, there is a unique diagonal matrix $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_K)$ minimizing $\|X - Z\Lambda\|_F$ given by

$$\lambda_j = \frac{(Z^\top X)_{jj}}{\|Z^j\|_2^2} \quad j = 1, \ldots, K.$$

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$$\lambda_j = \frac{(Z^\top X)_{jj}}{\|Z^j\|_2^2} \quad j = 1, \ldots, K.$$

It should be noted that Proposition 2 does not guarantee that Λ is invertible.

We now deal with *step 1, where $Q = R\Lambda$ is held fixed*.

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Recall that a matrix $X \in \mathcal{X}$ has the property that every row contains exactly one nonzero entry, and that every column is nonzero.

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Recall that a matrix $X \in \mathcal{X}$ has the property that every row contains exactly one nonzero entry, and that every column is nonzero.

The problem is to decide for each row, which column contains the nonzero entry.

After having found X, we rescale its columns so that $\|X\|_F = \|Z\|_F$.

For example, consider the following continuous solution and the discrete solution X:

$$\begin{pmatrix} 0.00 & -10.31 & 30.40 & 6.36 \\ 0.00 & -1.37 & 22.27 & -6.15 \\ -32.73 & -32.60 & -1.29 & 2.58 \\ 0.00 & -1.37 & 22.27 & -6.15 \\ 0.00 & 8.95 & 8.03 & -23.86 \\ -23.14 & -20.55 & -5.00 & -9.39 \\ 32.73 & -32.60 & -1.29 & 2.58 \\ 23.14 & -20.55 & -5.00 & -9.39 \\ -0.00 & -1.75 & -7.20 & -25.67 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

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\end{pmatrix}
\qquad
X = \begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}.
$$

We keep the leftmost largest entry on every row and set the others entries to 0.

Unfortunately, the matrix X may not be a correct solution, because the above prescription does not guarantee that every column of X is nonzero.

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When this happens, we *reassign certain nonzero entries in columns having "many" nonzero entries to zero columns, so that we get a matrix in $\mathcal{K}$*.

If we apply the method to the graph associated with the the matrix W_1 shown in Figure 3 for $K = 4$ clusters, the algorithm converges in 3 steps and we find the clusters shown in Figure 4.

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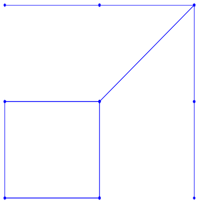

Figure 3: Underlying graph of the matrix W_1.

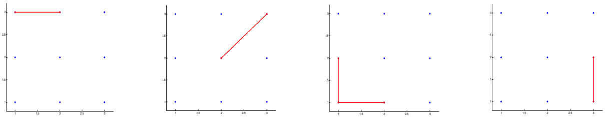

Figure 4: Four blocks of a normalized cut for the graph associated with W_1 .

The solution Z of the relaxed problem is

$$Z = \begin{pmatrix} -21.3146 & -0.0000 & 19.4684 & -15.4303 \\ -4.1289 & 0.0000 & 16.7503 & -15.4303 \\ -21.3146 & 32.7327 & -19.4684 & -15.4303 \\ -4.1289 & -0.0000 & 16.7503 & -15.4303 \\ 19.7150 & 0.0000 & 9.3547 & -15.4303 \\ -4.1289 & 23.1455 & -16.7503 & -15.4303 \\ -21.3146 & -32.7327 & -19.4684 & -15.4303 \\ -4.1289 & -23.1455 & -16.7503 & -15.4303 \\ 19.7150 & -0.0000 & -9.3547 & -15.4303 \end{pmatrix}.$$

We find the following sequence for $Q, Z * Q, X$:

$$Q = \begin{pmatrix} 0 & 0.6109 & -0.3446 & -0.7128 \\ -1.0000 & 0.0000 & 0.0000 & -0.0000 \\ 0.0000 & 0.5724 & 0.8142 & 0.0969 \\ -0.0000 & 0.5470 & -0.4672 & 0.6947 \end{pmatrix},$$

which is the initial Q obtained by method 1;

$$
Z * Q = \begin{pmatrix}
0.0000 & -10.3162 & 30.4065 & 6.3600 \\
0.0000 & -1.3742 & 22.2703 & -6.1531 \\
-32.7327 & -32.6044 & -1.2967 & 2.5884 \\
0.0000 & -1.3742 & 22.2703 & -6.1531 \\
0.0000 & 8.9576 & 8.0309 & -23.8653 \\
-23.1455 & -20.5505 & -5.0065 & -9.3982 \\
32.7327 & -32.6044 & -1.2967 & 2.5884 \\
23.1455 & -20.5505 & -5.0065 & -9.3982 \\
-0.0000 & -1.7520 & -7.2027 & -25.6776
\end{pmatrix}
$$

$$X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix};$$

$$Q = \begin{pmatrix} -0.0803 & 0.8633 & -0.4518 & -0.2102 \\ -0.6485 & 0.1929 & 0.1482 & 0.7213 \\ -0.5424 & 0.0876 & 0.5546 & -0.6250 \\ -0.5281 & -0.4581 & -0.6829 & -0.2119 \end{pmatrix}$$

$$
Z * Q = \begin{pmatrix}
-0.6994 & -9.6267 & 30.9638 & -4.4169 \\
-0.6051 & 4.9713 & 21.6922 & -6.3311 \\
-0.8081 & -6.7218 & 14.2223 & 43.5287 \\
-0.6051 & 4.9713 & 21.6922 & -6.3311 \\
1.4913 & 24.9075 & 6.8186 & -6.7218 \\
2.5548 & 6.5028 & 6.5445 & 31.3015 \\
41.6456 & -19.3507 & 4.5190 & -3.6915 \\
32.5742 & -2.4272 & -0.3168 & -2.0882 \\
11.6387 & 23.2692 & -3.5570 & 4.9716
\end{pmatrix}
$$

$$X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix};$$

$$Q = \begin{pmatrix} -0.3201 & 0.7992 & -0.3953 & -0.3201 \\ -0.7071 & -0.0000 & 0.0000 & 0.7071 \\ -0.4914 & -0.0385 & 0.7181 & -0.4914 \\ -0.3951 & -0.5998 & -0.5728 & -0.3951 \end{pmatrix}$$

$$
Z * Q = \begin{pmatrix}
3.3532 & -8.5296 & 31.2440 & 3.3532 \\
-0.8129 & 5.3103 & 22.4987 & -0.8129 \\
-0.6599 & -7.0310 & 3.2844 & 45.6311 \\
-0.8129 & 5.3103 & 22.4987 & -0.8129 \\
-4.8123 & 24.6517 & 7.7629 & -4.8123 \\
-0.7181 & 6.5997 & -1.5571 & 32.0146 \\
45.6311 & -7.0310 & 3.2844 & -0.6599 \\
32.0146 & 6.5997 & -1.5571 & -0.7181 \\
4.3810 & 25.3718 & -5.6719 & 4.3810
\end{pmatrix}
$$

$$X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

During the next round, the exact same matrices are obtained and the algorithm stops.

Any matrix obtained by flipping the signs of some of the columns of a solution ZR of problem $(*_2)$ is still a solution.

Any matrix obtained by flipping the signs of some of the columns of a solution ZR of problem $(*_2)$ is still a solution.

Moreover, all entries in X are nonnegative. It follows that a "good" solution ZQ_p (that is, close to a discrete solution) should have the property that the average of each of its column is nonnegative.

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We found that the following heuristic is quite helpful in finding a better discrete solution X:

Given a solution ZR of problem $(*_2)$, we compute ZQ_p, defined such that if the average of column $(ZR)^j$ is negative, then $(ZQ_p)^j = -(ZR)^j$, else $(ZQ_p)^j = (ZR)^j$.

Figure 5 shows a graph (on the left) and the graph drawings X and $Z * R$ obtained by applying our method for three clusters.

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The rows of X are represented by the red points along the axes, and the rows of $Z * R$ by the green points (on the right).

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The rows of X are represented by the red points along the axes, and the rows of $Z * R$ by the green points (on the right).

The original vertices corresponding to the rows of Z are represented in blue.

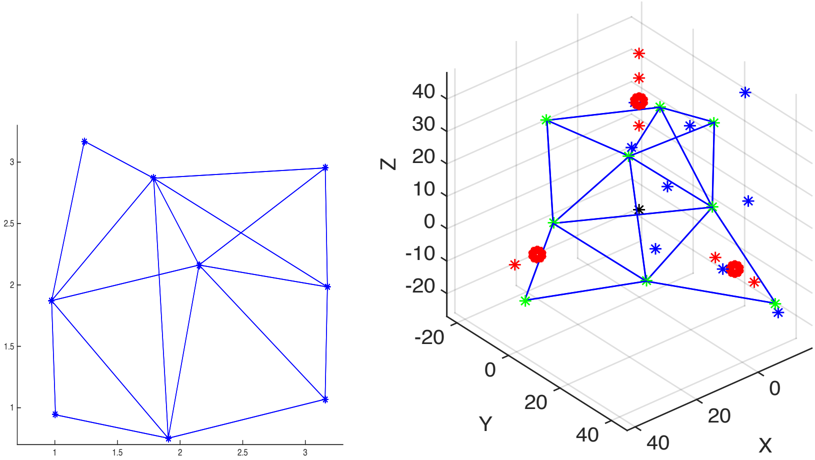

Figure 5: A graph and its drawing to find 3 clusters.

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It remains to initialize Q^* to start the process, and then steps (1) (holding Q fixed) and (2) (holding X fixed) are iterated, starting with step (1).

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Method 1. One method is to use an orthogonal matrix denoted R_1, such that distinct columns of ZR_1 are *simultaneously orthogonal and D-orthogonal*.

The matrix R_1 can be found by diagonalizing $Z^\top Z$ as $Z^\top Z = R_1 \Sigma R_1^\top$, as we explained earlier. We write $Z_2 = ZR_1$.

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We also have implemented various methods for improving the initial X.

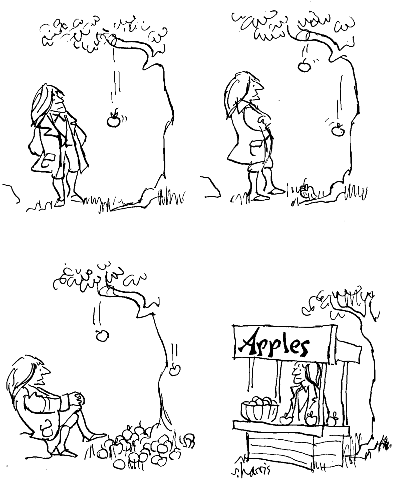

Figure 6: Newton goes to Wharton

6. Signed Graphs

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Weighted graphs for which the weight matrix is a symmetric matrix in which negative and positive entries are allowed are called *signed graphs*.

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The problem of clustering the nodes of a signed graph arises naturally as a generalization of the clustering problem for weighted graphs.

From our perspective, we would like to know whether clustering using normalized cuts can be extended to signed graphs.

Given a signed graph $G = (V, W)$ (where W is a symmetric matrix with zero diagonal entries), the *underlying graph* of G is the graph with node set V and set of (undirected) edges $E = \{\{v_i, v_j\} \mid w_{ij} \neq 0\}$.

Given the signed matrix

$$W = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & -1 & 1 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & -1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & -1 & 0 & 1 & 0 & -1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & -1 & -1 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & -1 & 0 \end{pmatrix}$$

the corresponding signed graph is

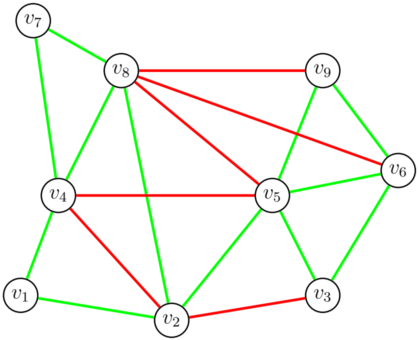

Figure 7: A signed graph G.

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A simple remedy is to use the *absolute values of the weights* in the degree matrix!

This idea applied to signed graph with weights $(-1, 0, 1)$ occurs in Hou. Kolluri, Shewchuk and O'Brien take the natural step of using absolute values of weights in the degree matrix in their original work on surface reconstruction from noisy point clouds.

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The trick of using absolute values of weights in the degree matrix allows the whole machinery that we have presented to be used to attack the problem of clustering signed graphs using normalized cuts.

This requires a modification of the notion of normalized cut.

If (V, W) is a signed graph, where W is an $m \times m$ symmetric matrix with zero diagonal entries and with the other entries $w_{ij} \in \mathbb{R}$ arbitrary, for any node $v_i \in V$, the *signed degree* of v_i is defined as

$$\overline{d}_i = \overline{d}(v_i) = \sum_{j=1}^{m} |w_{ij}|,$$

and the *signed degree matrix* $\overline{D}$ as

$$\overline{D} = \mathrm{diag}(\overline{d}(v_1), \ldots, \overline{d}(v_m)).$$

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For any subset A of the set of nodes V, let

$$\mathrm{vol}(A) = \sum_{v_i \in A} \overline{d}_i.$$

For any two subsets A and B of V, define $\mathrm{links}^+(A, B)$, $\mathrm{links}^-(A, B)$, and $\mathrm{cut}(A, \overline{A})$ by

$$\mathrm{links}^+(A, B) = \sum_{\substack{v_i \in A, v_j \in B \\ w_{ij} > 0}} w_{ij}$$

$$\mathrm{links}^-(A, B) = \sum_{\substack{v_i \in A, v_j \in B \\ w_{ij} < 0}} -w_{ij}$$

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Note that

$$\mathrm{cut}(A, \overline{A}) = \mathrm{links}^+(A, \overline{A}) + \mathrm{links}^-(A, \overline{A}).$$

Then, the *signed Laplacian* $\overline{L}$ is defined by

$$\overline{L} = \overline{D} - W,$$

and its normalized version $\overline{L}_{\mathrm{sym}}$ by

$$\overline{L}_{\mathrm{sym}} = \overline{D}^{-1/2}\, \overline{L}\, \overline{D}^{-1/2} = I - \overline{D}^{-1/2} W \overline{D}^{-1/2}.$$

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The signed Laplacian is symmetric positive semidefinite.

The signed Laplacian of the matrix W given earlier is

$$\overline{L} = \begin{pmatrix} 2 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 5 & 1 & 1 & -1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 3 & 0 & -1 & -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 5 & 1 & 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 1 & 6 & -1 & 0 & 1 & -1 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 2 & -1 & 0 \\ 0 & -1 & 0 & -1 & 1 & 1 & -1 & 6 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 0 & 1 & 3 \end{pmatrix}.$$

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The eigenvalues of $\overline{L}$ are

0.5175, 1.5016, 1.7029, 2.7058, 3.7284, 4.9604, 5.6026, 7.0888, 8.1921.

The matrix $\overline{L}$ is actually positive definite!

For any real $\lambda \in \mathbb{R}$, define $\mathrm{sgn}(\lambda)$ by

$$\mathrm{sgn}(\lambda) = \begin{cases} +1 & \text{if } \lambda > 0 \\ -1 & \text{if } \lambda < 0 \\ 0 & \text{if } \lambda = 0. \end{cases}$$

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Proposition 3

For any $m \times m$ symmetric matrix $W = (w_{ij})$, if we let $\overline{L} = \overline{D} - W$ where $\overline{D}$ is the signed degree matrix associated with W, then we have

$$x^\top \overline{L} x = \frac{1}{2} \sum_{i,j=1}^{m} |w_{ij}| (x_i - \mathrm{sgn}(w_{ij}) x_j)^2 \quad \text{for all } x \in \mathbb{R}^m.$$

Consequently, $\overline{L}$ is positive semidefinite.

7. Signed Normalized Cuts

As before, given a partition of V into K clusters $(A_1, \ldots, A_K)$, if we represent the jth block of this partition by a vector X^j such that

$$X_i^j = \begin{cases} a_j & \text{if } v_i \in A_j \\ 0 & \text{if } v_i \notin A_j, \end{cases}$$

for some $a_j \neq 0$, then we have the following result.

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Proposition 4

For any vector X^j representing the jth block of a partition $(A_1, \ldots, A_K)$ of V, we have

$$(X^j)^\top \overline{L} X^j = a_j^2(\mathrm{cut}(A_j, \overline{A_j}) + 2\mathrm{links}^-(A_j, A_j)).$$

Since with the revised definition of $\mathrm{vol}(A_j)$, we also have

$$(X^j)^\top \overline{D} X^j = a_j^2 \sum_{v_i \in A_j} \overline{d}_i = a_j^2 \mathrm{vol}(A_j),$$

we deduce that

$$\frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top \overline{D} X^j} = \frac{\mathrm{cut}(A_j, \overline{A_j}) + 2\mathrm{links}^-(A_j, A_j)}{\mathrm{vol}(A_j)}.$$

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The calculations of the previous paragraph suggest the following definition.

Definition 1

The *signed normalized cut* $\mathrm{sNcut}(A_1, \ldots, A_K)$ of the partition $(A_1, \ldots, A_K)$ is defined as

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A_j})}{\mathrm{vol}(A_j)} + 2 \sum_{j=1}^{K} \frac{\mathrm{links}^{-}(A_j, A_j)}{\mathrm{vol}(A_j)}.$$

Based on previous computations, we have

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top \overline{D} X^j}.$$

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where X is the $N \times K$ matrix whose jth column is X^j.

Therefore, *this is the same problem as in the unsigned case, with L replaced by $\overline{L}$ and D replaced by $\overline{D}$*.

Observe that minimizing $\mathrm{sNcut}(A_1, \ldots, A_K)$ amounts to

1. minimizing the number of positive and negative edges between clusters, and also
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The K-clustering problem for signed graphs is related but not equivalent to another problem known as *correlation clustering*.

In correlation clustering, in our terminology and notation, given a graph $G = (V, W)$ with positively and negatively weighted edges, one seeks a clustering of V that

1. minimizes the sum $\mathrm{links}^{-}(A_j, A_j)$ of the absolute values of the negative weights of the edges within each cluster A_j, and
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In contrast to K-clustering, the number K of clusters is not given in advance, and there is no normalization with respect to size of volume.

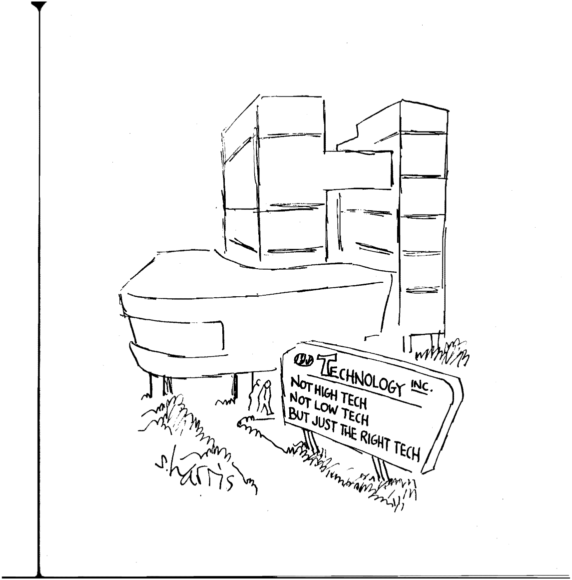


Figure 8: Just the right tech

8. Semantic Word Clusters

Finding sets of similar words is important for various Natural Language Processing (NLP) tasks. The desired similarity can be part-of-speech, tense, etc. and in our case we want closest semantic equivalence. For tasks such as machine translation, considering antonyms as equivalent is extremely problematic.

This is akin to thesaurus sets, but given the fact that language changes rapidly be changes in meaning, new words or spellings (especially for twitter), as well as multitudes of languages, we aim to have data driven clusters.

Semantic Word Cluster Problem

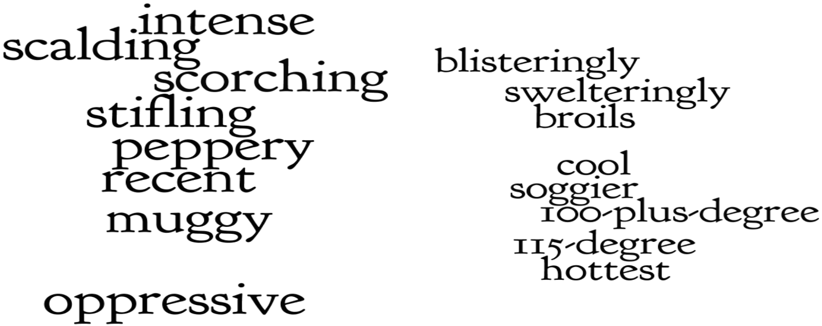


Figure 9: Thesaurus based (left) versus data-driven (right) clusters for “hot”. It is important to note **cool** on the right.

Representing Words as Vectors

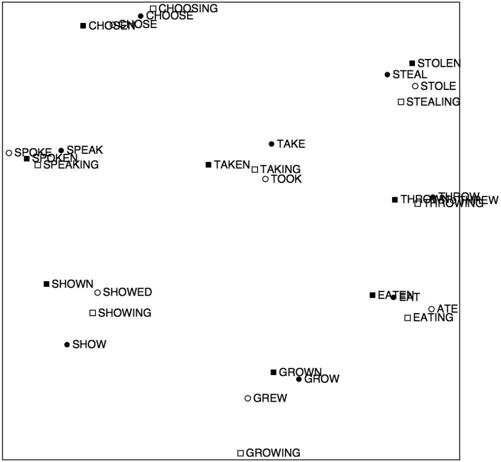
For word representations the initial obvious vector representation is a "one-hot" representations where word i is represented by a vector having all zeros for the size of our vocabulary aside from position i which is 1.

$$\begin{aligned} \text{hot} &= \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 \end{pmatrix}^\top \\ \text{scorching} &= \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}^\top \end{aligned}$$

However, in this representation all words are orthogonal, which is highly undesirable.
Instead, we use so called word embeddings, which are dense vector representations in $\mathbb{R}^D$ where D is much smaller than the vocabulary.

Representing Words as Vectors

$$\textit{shown} = \begin{pmatrix} 0.286 \\ 0.792 \\ -0.177 \\ -0.107 \\ 0.109 \\ -0.542 \\ 0.349 \\ 0.271 \end{pmatrix}$$



[Rohde et al. 2005. An Improved Model of Semantic Similarity Based on Lexical Co-Occurrence]

Representing Words as Vectors

The distributional hypothesis is that similar words are used in similar context (Harris 1954). Many vector popular representations (Eigenwords, GloVe, and word2vec) use adjacent words. However often antonyms such as "hot" and "cold" occur in similar contexts and thus have similar representations.

I meant... do I have time to fix you a **hot** lunch?
Tossing the **hot** pan holder on the counter, she untied the apron
He sipped the **hot** liquid and grimaced.
Her face felt **hot** again.
"Aren't you **cold**?" he asked
But, unfortunately, I struck my foot on a rock and fell forward into the **cold** water.

Table 1: "hot" and "cold" in sentence contexts [1] .

[1] from http://sentence.yourdictionary.com/

Embedding into Graph

We define the distance between two words $word_i$ and $word_j$ as $dist(word_i, word_j) = \|word_i - word_j\|$.
For the edge weight between two words

$$W_{ij} = \begin{cases} 0 & \text{if } e^{-\frac{dist(word_i, word_j)^2}{\sigma}} < thresh \\ e^{-\frac{dist(word_i, word_j)^2}{\sigma}} & \text{otherwise} \end{cases}.$$

We can represent the thesaurus as a matrix where

$$T_{ij} = \begin{cases} 1 & \text{if words } i \text{ and } j \text{ are synonyms} \\ -1 & \text{if words } i \text{ and } j \text{ are antonyms} \\ 0 & \text{otherwise} \end{cases}.$$

We can write the weight matrix of the signed graph as $\hat{W}_{ij} = T_{ij} W_{ij}$ or in matrix form $\hat{W} = T \odot W$ where $\odot$ denotes element-wise multiplication.

Embedding into Graph