Spectral K-Way Ratio-Cut Partitioning
Part I: Preliminary Results

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Abstract

Recent research on partitioning has focussed on the ratio-cut cost metric which maintains a balance between the sizes of the edges cut and the sizes of the partitions without fixing the size of the partitions a priori. Iterative approaches and spectral approaches to two-way ratio-cut partitioning have yielded higher quality partitioning results. In this paper we develop a spectral approach to multi-way ratio-cut partitioning which provides a generalization of the ratio-cut cost metric to k-way partitioning and a lower bound on this cost metric. Our approach uses Lanczos algorithm to find the k smallest eigenvalue/eigenvector pairs of the Laplacian of the graph. The eigenvectors are used to construct an orthogonal projection to map a vertex (of the graph) in an n-dimensional space into a k-dimensional subspace. We exploit the (near) orthogonality of the projected points to effect high quality clustering of points in a k-dimensional subspace. An efficient algorithm is presented for coercing the points in the k-dimensional subspace into k-partitions. Advancement over the current work is evidenced by the results of experiments on the standard MCNC benchmarks.

1 Introduction

We present a method for k-way partitioning based on spectral techniques by extending the techniques of Hagen and Kahng [1]. The k-way partition problem can be formulated as the search for a projection of n-dimensional space onto a k-dimensional subspace, mapping the n unit-vector basis (the n nodes of a graph) into k distinct points (the partitions) to minimize the weighted quadratic displacement. This is essentially the formulation given by Barnes [2, 3]. However, unlike Barnes' formulation we do not assume any pre-determined partition sizes.

By Hall's result [4], using the k eigenvectors of the graph's Laplacian, corresponding to the smallest k eigenvalues provides a projection which minimizes the weighted quadratic displacement under the orthonormality constraint. In the case of a partition, this amounts to the number of edges cut.

We show that a k projection provided by a partition can be reformulated as an orthonormal projection. This reformulation no longer minimizes the number of edges cut, but a new cost metric which incorporates the size of the partitions of a k-way partition $\mathcal{P} = \{P_1, P_2, \ldots P_k\}$:

$$cost(\mathcal{P}) = \sum_{h=1}^{k} \frac{E_h}{|P_h|}.$$

Here, E_h denotes the number of edges between nodes in partition P_h and nodes outside the partition. Interestingly, in the case of $k = 2$, this is the ratio-cut metric defined by Cheng and Wei scaled by the number of nodes in the graph [5]. The sum of the smallest k eigenvalues provides a lower bound on this cost metric.

A geometric interpretation of the eigenvectors provides a method for transforming the eigenvector solution into a partition. More significantly, this formulation provides a heuristic for identifying the *natural* number of partitions, k, *a priori*. Scaling the cost function above by $\frac{1}{k(k-1)}$ to offset the influence of k on this cost metric (fewer nodes per partition and higher expected degrees) provides a means of comparing partitions across different k's.

2 Definitions

Given an undirected graph G with n nodes, $v_1, v_2, \ldots, v_n$, the *adjacency matrix* of G is the $n \times n$ matrix $A(G) = [a_{ij}]$ defined by,

$$a_{ij} = \text{the number of edges between } v_i \text{ and } v_j.$$

If G is simple (no loops or parallel edges), then all of the entries in $A(G)$ are 1's or 0's and there are 0's along the diagonal. The *degree matrix* of G is the $n \times n$ matrix $D(G) = [d_{ij}]$

defined by,

$$d_{ij} = \begin{cases} degree(v_i) & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

The *Laplacian*[1]of G is the $n \times n$ matrix $Q(G) = D(G) - A(G)$.

A k-partition of the nodes of G, $\mathcal{P} = \{P_1, P_2, \ldots P_k\}$ is represented by an $n \times k$ *assignment matrix* $Y(\mathcal{P}) = [y_{ih}]$ where

$$y_{ih} = \begin{cases} 1 & \text{if } v_i \in P_h \\ 0 & \text{if } v_i \notin P_h \end{cases}$$

The rows of Y sum to 1 and column h sums to $|P_h|$.

A k-partition of G, $\mathcal{P} = \{P_1, P_2, \ldots P_k\}$ can also be represented by the $n \times n$ partition matrix[2] $P = [p_{ij}]$ where

$$p_{ij} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are in the same partition} \\ 0 & \text{otherwise} \end{cases}$$

Given a simple graph G and a partition of its nodes, $\mathcal{P}$, the *partition graph* $G_{\mathcal{P}}$ is the graph with k vertices $u_1, u_2, \ldots, u_k$ where the number of edges between u_g and u_h for $g \neq h$ is

$$\sum_{v_i \in P_g} \sum_{v_j \in P_h} a_{ij} = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} y_{ig} y_{jh},$$

where Y is the assignment matrix of $\mathcal{P}$. This is the graph whose nodes are the partitions and whose interconnections are inherited from the edges of G.

3 Graph partitioning and some basic properties of the Laplacian

Observation 1 *From Mohar "The Laplacian Spectrum of Graphs" [6]*

$$\sum_{i=1}^{n} \lambda_i = 2|E(G)| = \sum_{i=1} degree(v_i)$$

This follows from the Handshaking Lemma (the sum of the degrees of all nodes in an undirected graph is twice the number of edges) and the trace of a symmetric matrix (the sum of its diagonal entries) is the sum of its eigenvalues.

[1]aka *Kirchoff matrix* aka *admittance matrix*

[2]This was defined in Barnes' SIAM paper [2].

Observation 2 *If Y is an $n \times k$ matrix then $Y^TQ(G)Y$ is a $k \times k$ matrix whose gh^{th} component is*

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}-y_{jg})(y_{ih}-y_{jh}).$$

Proof: Since $Y^TQ(G)Y = Y^T(D(G)-A(G))Y = Y^TD(G)Y - Y^TA(G))Y$ the gh^{th} component of $Y^TQ(G)Y$ is

$$\begin{aligned}
\sum_{i=1}^{n} y_{ig}d_{ii}y_{ih} - \sum_{i=1}^{n} y_{ig}(\sum_{j=1}^{n} a_{ij}y_{jh}) &= \sum_{i=1}^{n} y_{ig}y_{ih}(\sum_{j=1}^{n} a_{ij}) - \sum_{i=1}^{n} y_{ig}(\sum_{j=1}^{n} a_{ij}y_{jh}) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{ih}) - \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{jh}) \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{ih}) - \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{jh}) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{ih}) \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{ih}) - \sum_{i=1}^{n}\sum_{j=1} na_{ij}(y_{ig}y_{jh}) + \frac{1}{2}\sum_{j=1}^{n}\sum_{i=1}^{n} a_{ji}(y_{jg}y_{jh}) \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{ih}) - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} 2a_{ij}(y_{ig}y_{jh}) + \frac{1}{2}\sum_{j=1}^{n}\sum_{i=1}^{n} a_{ij}(y_{jg}y_{jh}) \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}y_{ih} - 2y_{ig}y_{jh} + y_{jg}y_{jh}) \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}-y_{jg})(y_{ih}-y_{jh})
\end{aligned}$$

□

Observation 3 *If Y is the assignment matrix for $\mathcal{P}$ then $Y^TQ(G)Y = Q(G_{\mathcal{P}})$, the Laplacian of $G_{\mathcal{P}}$.*

Proof: First consider the g^{th} diagonal entry of $Y^TQ(G)Y$:

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}-y_{jg})^2.$$

Since Y is an assignment matrix, $a_{ij}(y_{ig}-y_{jg})^2$ will be 1 only when exactly one of v_i and v_j is in P_g and $a_{ij}=1$. Summed over all i and j this gives twice the total number of edges from nodes in P_g to nodes not in P_g. Hence the g^{th} diagonal entry is the degree of u_g in $G_{\mathcal{P}}$.

Now consider an off-diagonal entry ($h \neq g$). The gh^{th} component of $Y^TQ(G)Y$ is:

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(y_{ig}-y_{jg})(y_{ih}-y_{jh}).$$

Note that $y_{ig} - y_{jg}$ will be non-zero if and only if exactly one of v_i or v_j is in P_g. The same holds for $y_{ih} - y_{jh}$ with respect to P_h. Since a node can not be simultaneously in two partitions, $(y_{ig} - y_{jg})(y_{ih} - y_{jh})$ is non-zero exactly when one of v_i or v_j is in P_g and the other is in P_h. If this is the case and a_{ij} must be non-zero, then the ij^{th} term of the summation is -1. Hence summing over all i and j gives minus twice the number of edges between nodes in partition P_g and nodes in partition P_h. $\square$

Observation 4 *If P is a partition matrix, then its eigenvalues $\lambda(P) = \{m_1, m_2, ..., m_k\}$, where m_i is the number of nodes in the i^{th} partition (E. Barnes).*

Observation 5 *If Y is the assignment matrix for $\mathcal{P}$ then YY^T is the partition matrix.*

Proof: The ij^{th} element of YY^T is

$$\sum_{h=1}^{k} y_{ih} y_{jh}.$$

The term $y_{ih}y_{jh}$ will be 1 if and only if both v_i and v_j are in P_h, and hence the sum is 1 exactly when v_i and v_j are in the same partition and 0 otherwise. $\square$

Observation 6 *If Y is the assignment matrix for $\mathcal{P}$ then Y^TY is a diagonal matrix with $|P_g|$ in the g^{th}entry.*

Proof: The gh^{th} element of Y^TY is

$$\sum_{i=1}^{n} y_{ig} y_{ih}.$$

The term $y_{ig}y_{ih}$ can only be 0 when $h \neq g$ since node v_i can be in at most one of the two partitions. Hence the off-diagonal entries will be 0's. On the diagonal we have

$$\sum_{i=1}^{n} y_{ig}^2$$

which sums to the number of nodes in P_g. $\square$

The partition problem considered by Barnes and Donath,Hoffman was to solve for Y given k and $|P_1|, |P_2|, \ldots, |P_k|$, the sizes of the partitions [7].

4 Ratio-cut graph partitioning

Now consider modifying the definition of the partition matrix to take into account the size of the partitions. Specifically, a k-partition of the nodes of G, $\mathcal{P} = \{P_1, P_2, \ldots P_k\}$ is represented by an $n \times k$ *ratioed assignment matrix* $R(\mathcal{P}) = [r_{ih}]$ where

$$r_{ih} = \begin{cases} \frac{1}{\sqrt{|P_h|}} & \text{if } v_i \in P_h \\ 0 & \text{if } v_i \notin P_h \end{cases}$$

The rows no longer necessarily sum to 1 and column h now sums to $\sqrt{|P_h|}$.

Observation 7 *If R is the ratioed assignment matrix for $\mathcal{P}$ then the g^{th} diagonal entry of $R^T Q(G) R$ is the degree of u_g in $G_{\mathcal{P}}$ divided by $|P_g|$, and the gh^{th} off-diagonal entry is minus the number of edges between P_g and P_h divided by $\sqrt{|P_g| \cdot |P_h|}$.* □

Proof: By Observation 2 the g^{th} diagonal entry of $R^T Q(G) R$ is:

$$\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} (r_{ig} - r_{jg})^2.$$

Since R is a ratioed assignment matrix, $a_{ij}(r_{ig} - r_{jg})^2$ will be non-zero only when exactly one of v_i and v_j is in P_g and $a_{ij} = 1$. Summed over all i and j this gives twice the total number of edges from nodes in P_g to nodes not in P_g. Each non-zero $(r_{ig} - r_{jg})^2$ is

$$\left(\pm \frac{1}{\sqrt{|P_h|}} \right)^2 = \frac{1}{|P_h|}.$$

Hence the g^{th} diagonal entry is the degree of u_g in $G_{\mathcal{P}}$ divided by $|P_g|$.

Now consider an off-diagonal entry ($h \neq g$). The gh^{th} component of $R^T Q(G) R$ is:

$$\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} (r_{ig} - r_{jg})(r_{ih} - r_{jh}).$$

Note that $r_{ig} - r_{jg}$ will be non-zero if and only if exactly one of v_i or v_j is in P_g. The same holds for $r_{ih} - r_{jh}$ with respect to P_h. Since a node can not be simultaneously in two partitions, $(r_{ig} - r_{jg})(r_{ih} - r_{jh})$ is non-zero exactly when one of v_i or v_j is in P_g and the other is in P_h. If this is the case and a_{ij} is non-zero, then the ij^{th} term of the summation is

$$\frac{-1}{\sqrt{|P_g|}\sqrt{|P_h|}}.$$

Hence summing over all i and j gives minus twice the number of edges between nodes in partition P_g and nodes in partition P_h divided by $\sqrt{|P_g| \cdot |P_h|}$. □

Given a k-partition of G, the $n \times n$ ratioed partition matrix $P_R = [rp_{ij}]$ where

$$rp_{ij} = \begin{cases} \frac{1}{|P_g|} & \text{if } v_i \text{ and } v_j \text{ both belong to } P_g \\ 0 & \text{otherwise} \end{cases}$$

Observation 8 *If R is a ratioed assignment matrix for $\mathcal{P}$ then $RR^T = P_R$, the ratioed partition matrix.*

Proof: The ij^{th} element of RR^T is

$$\sum_{h=1}^{k} r_{ih} r_{jh}.$$

The term $r_{ih} r_{jh}$ will be non-zero if and only if both v_i and v_j are in P_h, hence the sum is $\frac{1}{|P_h|}$ when v_i and v_j are in the same partition and 0 otherwise. □

Observation 9 *If R is the ratioed assignment matrix for $\mathcal{P}$ then $R^T R$ is I_k, an identity matrix.*

Proof: The gh^{th} element of $R^T R$ is

$$\sum_{i=1}^{n} r_{ig} r_{ih}.$$

The term $r_{ig} r_{ih}$ can only be 0 when $h \neq g$ since node v_i can be in at most one of the two partitions. Hence the off-diagonal entries will be 0's. On the diagonal we have

$$\sum_{i=1}^{n} r_{ig}^2$$

which sums to 1 since there are $|P_g|$ non-zero terms which are all $\frac{1}{|P_g|}$. □

Hence the ratioed partition matrix meets the constraint $R^T R = I_k$.

5 Relation between the eigenvalues and ratio cuts

Define the k-way ratio cut cost metric of a k-partition $\mathcal{P}$ of G to be

$$cost(\mathcal{P}) = \sum_{h=1}^{k} \frac{degree(u_h)}{|P_h|}.$$

(Recall that u_h is the node in the partition graph corresponding to P_h so $degree(u_h)$ is the number of edges in G with exactly one endpoint in P_h.)

Observation 10 *If $k = 2$, $cost(\mathcal{P})$ is the ratio-cut cost metric defined by Wei and Cheng scaled by n, the number of nodes in the graph.*

Proof: If $k = 2$, and E_c is the number of edges cut in $\mathcal{P} = \{P_1, P_2\}$, then we have

$$\begin{aligned}
cost(\mathcal{P}) &= \frac{degree(u_1)}{|P_1|} + \frac{degree(u_2)}{|P_2|} \\
&= \frac{E_c}{|P_1|} + \frac{E_c}{|P_2|} \\
&= E_c \left(\frac{1}{|P_1|} + \frac{1}{|P_2|} \right) \\
&= E_c \frac{|P_1| + |P_2|}{|P_1| \cdot |P_2|} \\
&= E_c \frac{n}{|P_1| \cdot |P_2|} \\
&= n \frac{E_c}{|P_1| \cdot |P_2|}
\end{aligned}$$

□

Observation 11 *If R is the ratioed assignment matrix associated with $\mathcal{P}$, then $cost(\mathcal{P}) = trace(R^T Q(G) R)$.*

This follows from Observation 7.

Minimizing $cost(\mathcal{P})$, amounts to finding a ratioed assignment matrix which minimizes the sum of the diagonal entries of $R^T QR$.

Observation 12 *The $n \times k$ matrix which minimizes the $trace(Y^T Q(G) Y)$ subject to the constraint $Y^T Y = I_k$, is the $n \times k$ matrix whose k columns consist of the k eigenvectors of Q corresponding to the k smallest[3] eigenvalues of Q.*

Proof: If we take the partials with respect to the variables in Y of the g^{th} diagonal entry the matrix Lagrangian of $Y^T Q(G) Y - \lambda(Y^T Y - I_k)$, and equate them to zero, this constrains column g of Y to be an eigenvector; no other columns are constrained. Thus the minimal solution will consist of a k eigenvectors of Q. These k eigenvectors must be distinct to satisfy $Y^T Y = I_k$. If V is formed with any k eigenvectors of Q then $QV = V\Lambda_k$ where Λ_k is the diagonal matrix formed with the eigenvalues corresponding to the k eigenvectors in V. This means that

$$V^T QV = V^T V \Lambda_k = I_k \Lambda_k = \Lambda_k$$

and the sum of the diagonal entries of $V^T QV$ is the sum of the eigenvalues corresponding to the k eigenvectors in V. It follows that this sum is minimized by selecting the eigenvectors corresponding to the k smallest eigenvalues of Q. □

[3] Eigenvalues may be repeated but eigenvectors may not.

Observation 13 *The sum of the smallest k eigenvalues is a lower bound on the minimum $cost(\mathcal{P})$ of any k-partition of G.*

In the case $k = 2$, since $\lambda_1 + \lambda_2 = 0 + \lambda_2 = \lambda_2$ we obtain

$$\lambda_2 \leq cost(\mathcal{P}) = n \frac{E_c}{|P_1| \cdot |P_2|}$$

which amounts to the result of Hagen and Kahng [1]

$$\frac{\lambda_2}{n} \leq \frac{E_c}{|P_1| \cdot |P_2|}.$$

obviously not a tight upper bound for a graph with large number of nodes.

Observation 14 *By Fiedler's inequality [8],*

$$\lambda_2 \geq 2\mathcal{C}(1 - \cos(\pi/n)))$$

where $\mathcal{C}$ is a cut set of the graph G, an upper bound on the optimal ratio-cut partitioning is

$$\frac{\lambda_2}{2(n-1)(1 - \cos(\pi/n))}$$

6 A new k-way spectral ratio cut method

The problem of finding an assignment is solved as follows:

1. Calculate all or enough(?) eigenvalues of $Q(G)$.
2. Select k. See Section 7 below.
3. Find the eigenvectors corresponding to these k smallest eigenvalues.
4. Construct V, an $n \times k$ matrix whose columns are the k eigenvectors.
5. Compute $Z = VV^T$.
6. Construct a matrix $P = [p_{ij}]$ from Z where

$$p_{ij} = \begin{cases} 1 & \text{if } z_{ij} >= \frac{1}{n} \\ 0 & \text{otherwise} \end{cases}$$

   This is a heuristic of finding a partition using Z as "close" to P as possible. This method of coercing Z into a partition matrix doesn't always work. See Section 8 for alternatives.

7 Selecting the number of partitions k

In order to compare costs of partitions with different sizes, we scale our cost metric by $\frac{n}{k(k-1)}$,

$$scost(\mathcal{P}) = \frac{n \cdot cost(\mathcal{P})}{k(k-1)}.$$

The quantity $\frac{n}{k}$ is the average number of nodes in a balanced k-way partition and $k-1$ is the degree of a node in the complete graph with k nodes.

Observation 15 *For a random graph with edge probability f, and any partition $\mathcal{P}$ of size k,*

$$scost(\mathcal{P}) = fn \cdot \frac{n}{k}$$

which is a generalization of results of Cheng and Wei for bipartition [5]. (We are not sure yet what this means, may be this is the average degree of the partition graph per partition. But it will result in $k = n$ being selected, if the heuristics by eigenvalues estimation below is accurate).

We would like to select the k that produces the smallest $scost()$

$$\frac{n}{k(k-1)} \sum_{h=1}^{k} \frac{degree(u_h)}{|P_h|}$$

but since we do not know the optimal ratio-cut partition for any k we use the lower bound as an indicator. That is, we choose the k which minimizes

$$\frac{n}{k(k-1)} \sum_{h=1}^{k} \lambda_h$$

where $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ is the non-decreasing order of the eigenvalues of Q.
Note that this is a HEURISTIC.

8 Geometrical interpretation

The $n \times n$ matrix in $\mathbf{R}^k$, $RR^T = P_R$, the ratioed partition matrix is a *projector*, since $P_R^2 = P_R$.

The $n \times n$ matrix in $\mathbf{R}^k$

$$Z = VV^T$$

(which approximates the ratioed assignment matrix P_R) also forms an *orthogonal projection* of $\mathbf{R}^n$ spanned by the column vectors of Q onto a subspace of $\mathbf{R}^k$ spanned by the k smallest eigenvectors.

Observation 16 *Z has exactly k nonzero eigenvalues which are all 1, i.e.,*

$$\lambda(VV^T) = 1$$

Proof: Let the columns of the matrix $\mathbf{X}$ be the eigenvectors of Z, and Λ be their corresponding matrix of eigenvalues

$$\begin{aligned} VV^T\mathbf{X} &= \mathbf{X}\Lambda \\ V^TVV^T\mathbf{X} &= V^T\mathbf{X}\Lambda \\ I_k &= \Lambda \end{aligned}$$

□

Observation 17 *The nonzero eigenvalues of the ratioed partition matrix RR^T are all* `1`*s.*

Proof: Same as above. □

Observation 18 *The "distance" between the subspaces formed by ratioed assignment matrix R and V is given by Hoffman-Wielandt inequality and is bounded from below:*

$$||(RR^T) - (VV^T)||_2 \geq 0$$

Observation 19 *The distance between two equidimensional subspaces spanned by R and V is*

$$\sqrt{1 - \sigma^2_{min}(R^TV)}$$

where $\sigma_{min}(R^TV)$ is the smallest singular value of matrix R^TV (By **CS Decomposition**, Golub and van Loan, pg. 77). This is the generalized sine angle between the two subspaces.

The P_R matrix projects $\mathbf{R}^n$ onto the $\mathbf{R}^k$ subspace defined by the orthonormal R. If the n nodes of the graph G are associated with the n unit-vectors of $\mathbf{R}^n$, then nodes belonging to the same partition are mapped to the same point by R. Since P_R is "close" to the subspace defined by V^TV, the nodes belonging to the same partition should have "close" projections under V. This suggests a heuristic for constructing the R which is "closest" to V: use proximity of the images of the unit-vectors under V. In cases of ambiguity the distance can be verified.

9 Summary

We have presented some preliminary but new and basic results on spectral k-way ratio-cut partitioning in this report. The next report will demonstrate the effectiveness of this method and some experimental results.

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