Contemporary Mathematics
Volume 180, 1994

AN ANALYSIS OF SPECTRAL GRAPH PARTITIONING VIA QUADRATIC ASSIGNMENT PROBLEMS

ALEX POTHEN

ABSTRACT. Recently a spectral algorithm for partitioning graphs has been widely used in many applications including domain decomposition. Following some work of Rendl and Wolkowicz, we describe a mathematical programming formulation of the graph partitioning problem, and obtain lower bounds on the number of edges cut by a partition. We also show that finding a nearest feasible solution to the partitioning problem from an infeasible solution that attains the lower bound leads to a justification of the spectral algorithm.

1. INTRODUCTION

A fundamental problem in the solution of systems of equations by domain decomposition is the problem of partitioning the domain into a given number of subdomains, such that the subdomains have approximately equal amounts of work and few edges cross the subdomains. (Other criteria to measure the "communication" requirements may be used, but for simplicity we consider here only the number of edges.) This problem can be formulated as the problem of partitioning a graph into subsets of specified sizes such that few edges join different subsets. The graph partitioning problem has applications in other contexts such as the data- and task-mapping problem in parallel computation, the ordering problem in direct methods for sparse matrix factorization, etc.

A large number of methods have been proposed in recent years for the graph partitioning problem. Here we consider a widely-used spectral graph partitioning algorithm that was motivated by earlier work of Alan Hoffman, Miroslav Fiedler, Earl Barnes, Bojan Mohar, *inter alios*. The work in [6] showed that the spectral partitioning algorithm computes high-quality partitions for large finite element meshes; this paper also contains a brief survey of earlier work, and additional theoretical results. Since then the spectral method has been carefully implemented, extended, and employed to partition problems in several application contexts; for instance, [5, 7, 10, 11]. However, despite its good computational behavior, a sound theoretical justification of the method has been lacking.

In this paper we employ a mathematical programming formulation to obtain lower bounds on the number of edges cut by a partition, and to justify the spectral

---

1991 *Mathematics Subject Classification*. Primary 68R10, 65K05, 65Y05.

This work was supported by the National Science Foundation grant CCR-9024954, by the U. S. Department of Energy grant DE-FG02-91ER25095, and by the Canadian Natural Sciences and Engineering Research Council under grant OGP0008111 at the University of Waterloo.

This paper is in final form and no version of it will be submitted for publication elsewhere.

partitioning algorithm. The lower bounds are obtained by a projection technique for quadratic assignment problems (QAPs) developed by Hadley, Rendl, and Wolkowicz [4], and applied to the graph partitioning problem by Rendl and Wolkowicz [8], who formulated the problem in terms of the adjacency matrix (perturbed by a diagonal matrix). Computational results from their formulation are reported in [2]. The formulation of the bipartition problem is given here in terms of the Laplacian matrix, and although it is equivalent to the formulation with respect to the adjacency matrix (i.e., there is a choice of the diagonal perturbation that leads to the Laplacian eigenvalues), we believe this treatment is more direct and easier to understand. Due to space limitations, we do not provide extensive computational results here. None of these results are new; they can all be derived from the earlier results of Rendl and Wolkowicz [8].

The QAP formulation has also been applied to envelope-size minimization and the related 2-sum minimization problem [3]. Another justification for the spectral partitioning algorithm may be found in [1].

2. Bipartition and the quadratic assignment problem

Consider the problem of partitioning a graph $G = (V, E)$ into two subgraphs of m_1 and m_2 vertices such that the number of edges "cut", i.e., the number of edges joining one subgraph to the other, is minimized. We denote the two vertex subsets by V_1 and V_2, with $|V_j| = m_j$ for $j = 1$, 2, and $m_1 + m_2 = n$. This problem can be formulated as a quadratic assignment problem (QAP) involving the Laplacian matrix Q of the graph G. Recall that the Laplacian $Q = D - A$, where D is a diagonal matrix of vertex-degrees, and A is the adjacency matrix of G.

2.1. Formulation of bipartition as a QAP. Let $X = \begin{pmatrix} \underline{x}_1 & \underline{x}_2 \end{pmatrix}$ be an $n \times 2$ *partition matrix* consisting of the two indicator vectors $\underline{x}_j$ (for $j = 1$, 2), where x_{ij} is equal to one if vertex i belongs to the set V_j, and is zero otherwise. Then

$$\underline{x}_j{}^T Q \underline{x}_j = \sum_{i=1}^{n} \sum_{k=1}^{n} x_{ij} q_{ik} x_{kj} = \sum_{v \in V_j} d(v) - 2|E(V_j, V_j)|,$$

where $d(v)$ is the number of vertices adjacent to v, and $E(V_j, V_j)$ is the set of edges in E with both endpoints in V_j. We denote the edges joining V_1 and V_2 by the set $\delta(V_1, V_2)$, and recall that the *trace* of a square matrix Q, denoted by $tr\ Q$, is the sum of its diagonal elements. Then

$$\begin{aligned} tr\ X^T Q X &= \sum_{v \in V} d(v) - 2|E(V_1, V_1)| - 2|E(V_2, V_2)| \\ &= 2|E| - 2|E(V_1, V_1)| - 2|E(V_2, V_2)| = 2|\delta(V_1, V_2)|. \end{aligned} \tag{1}$$

Thus the problem of minimizing the number of edges cut by a bipartition with part sizes equal to m_1 and m_2 can be written as

(2)
$$|\delta_{min}(V_1, V_2)| \equiv \min\{|\delta(V_1, V_2)| : |V_1| = m_1, |V_2| = m_2\} = (1/2) \min_X tr\ X^T Q X,$$

where X varies over partition matrices with exactly m_j ones in the jth column.

Let $\underline{u}_n = (1/\sqrt{n})\begin{pmatrix} 1 & 1 & \cdots & 1 \end{pmatrix}^T$ denote the n-vector of all ones, scaled to have 2-norm one. (We will write $\underline{u}$ instead of $\underline{u}_n$ when the dimension is clear from the context.) A partition matrix X is characterized by the following three conditions:

$$\begin{aligned}
&(3) \qquad & X\underline{u}_2 &= \sqrt{(n/2)}\,\underline{u}_n; \quad X^T\underline{u}_n = (1/\sqrt{n})\begin{pmatrix} m_1 \\ m_2 \end{pmatrix}; \\
&(4) \qquad & X^TX &= \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \equiv M; \\
&(5) \qquad & x_{ij} &\geq 0 \quad \text{for } i = 1, \dots, n; j = 1, 2.
\end{aligned}$$

The first part of the first condition states that each row sum of a partition matrix is one, signifying that each vertex belongs to exactly one of the parts V_1 or V_2. The second part shows that there are m_j vertices in the jth part V_j. The second condition indicates that the columns of a partition matrix are orthogonal, and the third that the elements of a partition matrix are nonnegative.

Scaling $X = YM^{1/2}$ simplifies the following exposition and exposes the structure of the problem. With this scaling, the conditions on X are transformed to the following conditions on Y:

$$\begin{aligned}
&(6) \qquad & Y\underline{m} &= \underline{u}_n; \qquad Y^T\underline{u}_n = \underline{m}, \quad \text{where } \underline{m} = (1/\sqrt{n})\begin{pmatrix} \sqrt{m_1} \\ \sqrt{m_2} \end{pmatrix}; \\
&(7) \qquad & Y^TY &= I_2; \\
&(8) \qquad & \left(YM^{1/2}\right)_{ij} &\geq 0 \quad \text{for } i = 1, \dots, n; j = 1, 2.
\end{aligned}$$

The objective function $tr\ X^TQX$ becomes $tr\ M^{1/2}Y^TQYM^{1/2} = tr\ MY^TQY$. In the last transformation we have used the identity $tr\ MN = tr\ NM$, where M is $n \times k$, and N is $k \times n$.

Minimizing this objective function subject to these constraints is NP-complete. Hence we obtain lower bounds on the number of edges cut by relaxing the third of these conditions.

2.2. Projected lower bounds. It is convenient to impose (6) on Y by projecting the problem to the subspace orthogonal to the manifold defined by this condition. Note that the two parts of this condition yield $YY^T\underline{u}_n = \underline{u}_n$, and $Y^TY\underline{m} = \underline{m}$. Thus we find that $\underline{m}$ is a right singular vector and that $\underline{u}_n$ is a left singular vector of Y corresponding to the singular value one. Choose an $n \times n$ orthogonal matrix $P_1 = \begin{pmatrix} \underline{u} & V \end{pmatrix}$, and a 2×2 orthogonal matrix $P_2 = \begin{pmatrix} \underline{m} & \underline{v} \end{pmatrix}$. The first step of the singular value decomposition of Y is

$$\begin{aligned}
P_1^TYP_2 &= \begin{pmatrix} \underline{u}^TY\underline{m} & \underline{u}^TY\underline{v} \\ V^TY\underline{m} & V^TY\underline{v} \end{pmatrix} = \begin{pmatrix} \underline{u}^T\underline{u} & \underline{m}^T\underline{v} \\ V^T\underline{u} & V^TY\underline{v} \end{pmatrix} \\
(9) \qquad &= \begin{pmatrix} 1 & 0 \\ \underline{0} & \underline{z} \end{pmatrix}, \quad \text{where } \underline{z} \equiv V^TY\underline{v}.
\end{aligned}$$

Thus if we choose Y to be

$$(10) \qquad Y = P_1\begin{pmatrix} 1 & 0 \\ \underline{0} & \underline{z} \end{pmatrix}P_2^T = \underline{u}\,\underline{m}^T + V\underline{z}\,\underline{v}^T,$$

then (6) is satisfied.

Substitution of this representation of Y in the orthogonality condition (7), followed by pre-multiplication with P_2^T and post-multiplication with P_2, shows that

$$\begin{pmatrix} 1 & 0 \\ 0 & \underline{z}^T \underline{z} \end{pmatrix} = I_2,$$

and hence we obtain the condition $\underline{z}^T \underline{z} = 1$.

Substituting for Y from (10) in the objective function $tr\, MY^TQY$, we find that since $Q\underline{u} = \underline{0}$, only one of the four terms survives, and it becomes

$$\begin{aligned} tr\, MY^TQY &= tr\, M\underline{v}\,\underline{z}^T V^T QV \underline{z}\,\underline{v}^T = tr\, \underline{v}^T M \underline{v}\, \underline{z}^T \widehat{Q} \underline{z} \\ &= (\underline{v}^T M \underline{v})\ (\underline{z}^T \widehat{Q} \underline{z}), \end{aligned} \tag{11}$$

where $\widehat{Q} \equiv V^TQV$ is the projected Laplacian.

The first term on the right-hand-side, $\underline{v}^T M \underline{v}$, is easily computed to be $2m_1m_2/n$, since $\underline{m} = (1/\sqrt{n})\begin{pmatrix} \sqrt{m_1} \\ \sqrt{m_2} \end{pmatrix}$ implies that $\underline{v} = \pm(1/\sqrt{n})\begin{pmatrix} \sqrt{m_2} \\ -\sqrt{m_1} \end{pmatrix}$. Thus we obtain the result $|\delta(V_1, V_2)| = (1/2)\ (2m_1m_2/n)\ \underline{z}^T \widehat{Q} \underline{z}$.

The bipartition problem is hence

$$\begin{aligned} |\delta_{min}(V_1, V_2)| &= (m_1m_2/n) \min_{\underline{z}} \underline{z}^T \widehat{Q} \underline{z} \\ \text{subject to} \quad & \underline{z}^T \underline{z} = 1, \\ & \left(\underline{u}\,\underline{m}^T M^{1/2} + V\underline{z}\,\underline{v}^T M^{1/2}\right)_{ij} \geq 0. \end{aligned} \tag{12}$$

Though this problem is intractable, a lower bound may be obtained by relaxing the second constraint, and thus we find

$$|\delta_{min}(V_1, V_2)| \geq (m_1m_2/n)\lambda_1(\widehat{Q}) = (m_1m_2/n)\lambda_2(Q), \tag{13}$$

since the eigenvalues of $\widehat{Q}$ are the $n-1$ nonzero eigenvalues of Q. The lower bound is attained by the corresponding eigenvector $\underline{z}_0 = V^T \underline{x}_2$, where $\underline{x}_2$ is the second Laplacian eigenvector. Hence the orthogonal matrix attaining the lower bound is

$$Y_0 = \underline{u}\,\underline{m}^T + VV^T \underline{x}_2\, \underline{v}^T. \tag{14}$$

2.3. Diagonal perturbations. The lower bound on the number of cut edges can be improved further by considering diagonal perturbations of the Laplacian. Let $Q(\underline{d}) = Q + Diag(\underline{d})$, where $\underline{d}$ is an n-vector whose components sum to zero. It can be verified that $tr\, X^TQ(\underline{d})X = tr\, X^TQX$, so that this perturbation has no effect on the number of cut edges. Proceeding as in the unperturbed case, we can show that

$$\begin{aligned} |\delta_{min}(V_1, V_2)| \geq\ & \max_{\underline{d}} \min_{\underline{z}} \Big\{ (m_1m_2/n)\underline{z}^T \widehat{Q}(d) \underline{z} \\ &+ (1/2n\sqrt{n})(m_1 - m_2)\sqrt{m_1m_2}\, \underline{d}^T\, \underline{z} \Big\}, \\ \text{subject to} \quad & \underline{z}^T \underline{z} = 1. \end{aligned} \tag{15}$$

The lower bound can be computed by nondifferentiable optimization techniques [9].

The lower bounds in terms of the unperturbed Laplacian are still weak for "well-shaped" finite-element meshes that possess partitions with few edges being cut. It would be interesting to see how much the bounds improve when diagonal perturbations are included.

2.4. Closest partition matrix. Which partition matrix Z is "closest" to the orthogonal matrix $X_0 = Y_0 M^{1/2}$ attaining the lower bound (see (14)) in the bipartition problem? We can answer this question by considering the objective function of the bipartition problem, which we may write as

$$\min_Z \, tr\, Z^T(Q+\alpha I)Z = \min_Z \, \|(Q+\alpha I)^{1/2} Z\|_F{}^2. \tag{16}$$

Here we have shifted the Laplacian by a small positive multiple of the identity to make the matrix $Q+\alpha I$ positive definite, so that its square root is nonsingular. This is necessary to obtain a weighted norm. It can be verified that this shifts the objective function by the constant $\alpha\, n$, and hence has no effect on the minimizer. We now expand Z about X_0 to obtain

$$\begin{aligned} &\min_Z \, \|(Q+\alpha I)^{1/2}\,(X_0 + (Z - X_0))\,\|_F{}^2 \\ = \;& \min_Z \, \|(Q+\alpha I)^{1/2} X_0\|_F{}^2 + 2\, tr\, X_0^T (Q+\alpha I)(Z - X_0) \\ + \;& \|(Q+\alpha I)^{1/2}(Z - X_0)\|_F{}^2. \end{aligned} \tag{17}$$

Here we have used the identity

$$\|A+B\|_F{}^2 = \|A\|_F{}^2 + \|B\|_F{}^2 + 2\, tr\, A^T B,$$

for real matrices A and B.

On the right-hand-side of (17), the first term is a constant since X_0 is a fixed orthogonal matrix; we ignore the third term, which is a quadratic in the difference $(Z - X_0)$, to obtain a linear approximation. Hence we consider the problem

$$\min_Z \, tr\, X_0^T(Q+\alpha I)Z \quad = \quad \min_Z \, tr\, M^{1/2} Y_0^T (Q+\alpha I) Z. \tag{18}$$

Substituting for Y_0 from (14), and noting that $\underline{u}^T Q = \underline{0}^T$, the problem becomes

$$\min_Z \, tr\, M^{1/2}\left(\underline{v}\,\underline{x}_2{}^T V V^T Q Z + \alpha\, \underline{m}\, \underline{u}^T Z + \alpha\, \underline{v}\, \underline{x}_2{}^T V V^T Z\right). \tag{19}$$

The second term in the right-hand-side is constant since $\underline{u}^T Z = (1/\sqrt{n})\begin{pmatrix} m_1 & m_2 \end{pmatrix}$ (by (3)), and hence the problem reduces to

$$\min_Z tr\, M^{1/2} \underline{v}\, \underline{x}_2{}^T V V^T (Q+\alpha I) Z. \tag{20}$$

Replacing $VV^T = P_1 P_1^T - \underline{u}\,\underline{u}^T = (I_n - \underline{u}\,\underline{u}^T)$, noting again that $\underline{u}$ is an eigenvector of Q corresponding to the zero eigenvalue (or that $\underline{x}_2{}^T \underline{u} = 0$), the objective function simplifies to

$$\min_Z \, tr\, M^{1/2} \underline{v}\, \underline{x}_2{}^T (Q+\alpha I) Z = \min_Z \, (\lambda_2(Q) + \alpha)\, tr\, M^{1/2} \underline{v}\, \underline{x}_2{}^T Z.$$

Further simplifications are possible. An important observation is that in the bipartition problem $Z = \begin{pmatrix} \underline{z}_1 & \sqrt{n}\underline{u} - \underline{z}_1 \end{pmatrix}$, where $\underline{z}_1$ is an indicator vector with m_1 ones and remaining elements equal to zeros, and the second column of Z is the complement of $\underline{z}_1$ with respect to the vector of all ones. Also note that $M^{1/2}\underline{v} = \pm\sqrt{m_1 m_2/n}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. Putting these observations together, the problem becomes

$$\begin{aligned} & \left((\lambda_2(Q)+\alpha)\sqrt{m_1 m_2/n}\right) \min_{\underline{z}_1} tr \pm \begin{pmatrix} \underline{x}_2^T \underline{z}_1 & \underline{x}_2^T(\sqrt{n}\underline{u} - \underline{z}_1) \\ -\underline{x}_2^T \underline{z}_1 & -\underline{x}_2^T(\sqrt{n}\underline{u} - \underline{z}_1) \end{pmatrix} \\ (21) \quad = & \left(2(\lambda_2(Q)+\alpha)\sqrt{m_1 m_2/n}\right) \min_{\underline{z}_1} \pm \underline{x}_2^T \underline{z}_1. \end{aligned}$$

In going from the first to the second line we have used $\underline{x}_2^T\, \underline{u} = 0$.

Thus the algebraic manipulations in this subsection come to a glorious conclusion! One solution to (21), and hence to a linear approximation to the nearest partition matrix problem, is obtained by choosing $\underline{z}_1$ to have ones in rows corresponding to the smallest (most negative) m_1 eigenvector components of $\underline{x}_2$. A second solution is obtained by choosing the rows corresponding to the largest (most positive) m_1 eigenvector components. (These two solutions correspond to the choice of the sign in (21).) Hence we obtain a justification of the spectral algorithm for the bipartition problem which partitions the graph with respect to the m_1th smallest or largest second eigenvector component.

Acknowledgments. I thank Professor Stan Eisenstat of Yale University for his comments and questions, and for pointing out errors in a draft of this paper.

REFERENCES

1. T. F. Chan and W. K. Szeto. *On the near optimality of the recursive spectral bisection method for graph partitioning.* Manuscript, Feb. 1993.
2. J. Falkner, F. Rendl, and H. Wolkowicz. *A computational study of graph partitioning.* Math. Programming, 1994. To appear.
3. A. George and A. Pothen. *An analysis of the spectral approach to envelope reduction via a quadratic assignment formulation.* In preparation, 1994.
4. S.W. Hadley, F. Rendl, and H. Wolkowicz. *A new lower bound via projection for the quadratic assignment problem.* Mathematics of Operations Research, **17**(1992), 727–739.
5. B. Hendrickson and R. Leland. *An improved spectral graph partitioning algorithm for mapping parallel computations.* Technical Report SAND92-1460, UC-405, Sandia Natl. Lab., Albuquerque, N.M., Sep. 1992.
6. A. Pothen, H. D. Simon, and K. P. Liou. *Partitioning sparse matrices with eigenvectors of graphs.* SIAM J. Matrix Anal. Appl., **11**(1990), 430–452.
7. A. Pothen and L. Wang. *An improved spectral nested dissection algorithm.* In preparation, 1994.
8. F. Rendl and H. Wolkowicz. *A projection technique for partitioning the nodes of a graph.* Annals of Operations Research, 1994. This paper was written in 1990, and will appear in a special issue devoted to APMOD93.
9. H. Schramm and J. Zowe. *A version of the bundle idea for minimizing a nonsmooth function: Conceptual idea, convergence analysis, numerical results.* SIAM J. Opt., **2**(1992), 121–152.
10. H. D. Simon. *Partitioning of unstructured problems for parallel processing.* Computing Systems in Engineering, **2**(1991), 135–148.
11. Lie Wang. *Spectral Nested Dissection.* Ph.D. thesis, The Pennsylvania State University, University Park, PA, 1994.

COMPUTER SCIENCE DEPARTMENT, OLD DOMINION UNIVERSITY, NORFOLK, VA 23529-0162, AND ICASE, MS 132C, NASA-LARC, HAMPTON, VA 23681-0001.

E-mail address: pothen@icase.edu