AN ANALYSIS OF SPECTRAL ENVELOPE-REDUCTION VIA QUADRATIC ASSIGNMENT PROBLEMS*

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Abstract. A new spectral algorithm for reordering a sparse symmetric matrix to reduce its envelope size was described in [2]. The ordering is computed by associating a Laplacian matrix with the given matrix and then sorting the components of a specified eigenvector of the Laplacian. In this paper we provide an analysis of the spectral envelope reduction algorithm. We describe related 1- and 2-sum problems; the former is related to the envelope size, while the latter is related to an upper bound on the work in an envelope Cholesky factorization. We formulate the latter two problems as quadratic assignment problems, and then study the 2-sum problem in more detail. We obtain lower bounds on the 2-sum by considering a relaxation of the problem, and then show that the spectral ordering finds a permutation matrix closest to an orthogonal matrix attaining the lower bound. This provides stronger justification of the spectral envelope reduction algorithm than previously known. The lower bound on the 2-sum is seen to be tight for reasonably "uniform" finite element meshes. We show that problems with bounded separator sizes also have bounded envelope parameters.

Key words. 1-sum problem, 2-sum problem, envelope reduction, eigenvalues of graphs, Laplacian matrices, quadratic assignment problems, reordering algorithms, sparse matrices.

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1. Introduction. We provide a *raison d'être* for a novel spectral algorithm to reduce the envelope of a sparse, symmetric matrix, described in a companion paper [2]. The algorithm associates a discrete Laplacian matrix with the given symmetric matrix, and then computes a reordering of the matrix by sorting the components of an eigenvector corresponding to the smallest nonzero Laplacian eigenvalue. The results in [2] show that the spectral algorithm can obtain significantly smaller envelope sizes compared to other currently used algorithms. All previous envelope-reduction algorithms (known to us), such as the reverse Cuthill-McKee (RCM) algorithm and variants [3, 16, 17, 26, 37], are combinatorial in nature, employing breadth-first-search to compute the ordering. In contrast, the spectral algorithm is an algebraic algorithm whose good envelope-reduction properties are somewhat intriguing and poorly understood.

We describe problems related to envelope-reduction called the 1- and 2-sum problems, and then formulate these latter problems as quadratic assignment problems (QAPs). We show that the QAP formulation of the 2-sum enables us to obtain lower bounds on the 2-sum (and related envelope parameters) based on the Laplacian eigenvalues. The lower bounds seem to be quite tight for finite element problems when the mesh points are nearly all of the same degree, and the geometries are simple. Further, a closest permutation matrix to an orthogonal matrix that attains the lower bound is obtained, to within a linear approximation, by sorting the second Laplacian eigenvector components in monotonically increasing or decreasing order. This justifies the spectral envelope-reducing algorithm more strongly than earlier results.

Although initially envelope-reducing orderings were developed for use in envelope schemes for sparse matrix factorization, these orderings have been used in the past few years in several other applications. The RCM ordering has been found to be an effective pre-ordering in computing incomplete factorization preconditioners for preconditioned conjugate-gradient methods [4, 6]. Envelope-reducing orderings have been used in frontal methods for sparse matrix factorization [7].

The wider applicability of envelope-reducing orderings prompts us to take a fresh look at the reordering algorithms currently available, and to develop new ordering algorithms. Spectral envelope-reduction algorithms seem to be attractive in this context, since they
(i) compare favorably with existing algorithms in terms of the quality of the orderings [2],
(ii) extend easily to problems with weights, e.g., finite element meshes arising from discretizations of anisotropic problems, and
(iii) are fairly easily parallelizable.
Spectral algorithms are more expensive than the other algorithms currently available. But since the envelope-reduction problem requires only one eigenvector computation (to low precision), we believe the costs are not impractically high in computation-intensive applications, e.g., frontal methods for factorization. In contexts where many problems having the same structure must be solved, a substantial investment in finding a good ordering might be justified, since the cost can be amortized over many solutions. Improved algorithms that reduce the costs are being designed as well [25].

We focus primarily on the class of finite element meshes arising from discretizations of partial differential equations. Our goals in this project are to develop efficient software implementing our algorithms, and to prove results about the quality of the orderings generated.

The projection approach for obtaining lower bounds of a QAP is due to Hadley, Rendl, and Wolkowicz [19], and this approach has been applied to the graph partitioning problem by the latter two authors [35]. In earlier work a spectral approach for the graph (matrix) partitioning problem has been employed to compute a spectral nested dissection ordering for sparse matrix factorization, for partitioning computations on finite element meshes on a distributed-memory multiprocessor [21, 33, 34, 36], and for load-balancing parallel computations [22]. The spectral approach has also been used to find a pseudo-peripheral node [18]. Juvan and Mohar [23, 24] have provided a theoretical study of the spectral algorithm for reducing p-sums, where $p = 1$, 2, and ∞, and Helmberg et al. [20] obtain spectral lower bounds on the bandwidth. A survey of some of these earlier results may be found in [31]. Paulino et al. [32] have also considered the use of spectral envelope-reduction for finite element problems.

The following is an outline of the rest of this paper. In Section 2 we describe various parameters of a matrix associated with its envelope, introduce the envelope size and envelope work minimization problems, and the related 1- and 2-sum problems. We prove that bounds on the minimum 1-sum yield bounds on the minimum envelope size, and similarly, bounds on the minimum 2-sum yield bounds on the work in an envelope Cholesky factorization. We also show in this section that minimizing the 2-sum is NP-complete. We compute lower bounds for the envelope parameters of a sparse symmetric matrix in terms of the eigenvalues of the Laplacian matrix in Section 3. The popular RCM ordering is obtained by reversing the Cuthill-McKee (CM) ordering; the RCM ordering can never have a larger envelope size and work than the CM ordering, and is usually significantly better. We prove that reversing an ordering can improve or impair the envelope size by at most a factor Δ, and the envelope work by at most Δ^2, where Δ is the maximum degree of a vertex in the adjacency graph. In Section 4, we formulate the 2- and 1-sum problems as quadratic assignment problems. We obtain lower and upper bounds for the 2-sum problem in terms of the eigenvalues of the Laplacian matrix in Section 5 by means of a projection approach that relaxes a permutation matrix to an orthogonal matrix with row and column sums equal to one. We justify the spectral envelope-reduction algorithm in Section 6 by proving that a closest permutation matrix to an orthogonal matrix attaining the lower bound for the 2-sum is obtained, to within a linear approximation of the problem, by permuting the second Laplacian eigenvector in monotonically increasing or decreasing order. In Section 7 we show that graphs with small separators have small envelope parameters as well, by considering a modified nested dissection ordering. We present computational results in Section 8 to illustrate that the 2-sums obtained by the spectral reordering algorithm can be close to optimal for many finite element meshes. Section 9 contains our concluding remarks. The Appendix contains some lower bounds for the more general p-sum problem, where $1 \leq p < \infty$.

2. A menagerie of envelope problems.

2.1. The envelope of a matrix. Let A be an $n \times n$ symmetric matrix with elements a_{ij}, whose diagonal elements are nonzero. Various parameters of the matrix A associated with its envelope are defined below.

We denote the column indices of the nonzeros in the lower triangular part of the ith row by

$$\text{row}(i) = \{j : a_{ij} \neq 0 \text{ and } 1 \leq j \leq i\}.$$

For the ith row of A we define

$$\begin{aligned} f_i(A) &= \min\{j : j \in \text{row}(i)\}, \quad \text{and} \\ r_i(A) &= i - f_i(A). \end{aligned}$$

Here $f_i(A)$ is the column index of the first nonzero in the ith row of A (by our assumption of nonzero diagonals, $1 \leq f_i \leq i$), and the parameter $r_i(A)$ is the *row-width* of the ith row of A. The *bandwidth* of A is the maximum row-width

$$\text{bw}(A) = \max\{r_i(A) : i = 1, \ldots, n\}.$$

The *envelope* of A is the set of index pairs

$$\text{Env}(A) = \{(i,j) : f_i(A) \leq j < i, \; i = 1, \ldots, n\}.$$

For each row, the column indices lie in an interval beginning with the column index of the first nonzero element and ending with (but not including) the index of the diagonal nonzero element.

We denote the size of the envelope by $\text{Esize}(A) = |\text{Env}(A)|$. (The number $\text{Esize}(A) + n$ (which includes the diagonal elements) is called the *profile* of A [7].) The work in the Cholesky factorization of A that employs an envelope storage scheme is bounded from above by

$$\text{Wbound}(A) \equiv (1/2) \sum_{i=2}^{n} r_i(r_i + 3).$$

This bound is tight [29] when an ordering satisfies (1) $f_i(A) \leq f_j(A)$ when $i < j$ for all i, j between 1 and n, and (2) $f_i(A) < i$, for all $i = 2, \ldots, n$.

A 3×3 7-point grid and the nonzero structure of the corresponding matrix A are shown in Figure 2.1. A ' $\bullet$ ' indicates a nonzero element, and a ' $*$ ' indicates a zero element that belongs to the lower triangle of the envelope in the matrix. The row-widths given in Table 2.1 are easily verified from the structure of the matrix. The envelope size is obtained by summing the row-widths, and is equal to 24. (Column-widths c_i are defined later in this section.)

The values of these parameters strongly depend on the choice of an ordering of the rows and columns. Hence we consider how these parameters vary over symmetric permutations $P^T AP$ of a matrix A, where P is a permutation matrix. We define $\text{Esize}_{\min}(A)$, the minimum envelope size of A, to be the minimum envelope size among all permutations $P^T AP$ of A. The quantities $\text{Wbound}_{\min}(A)$ and $\text{bw}_{\min}(A)$ are defined in similar fashion. Minimizing the envelope size and the bandwidth of a matrix are NP-complete problems [28], and minimizing

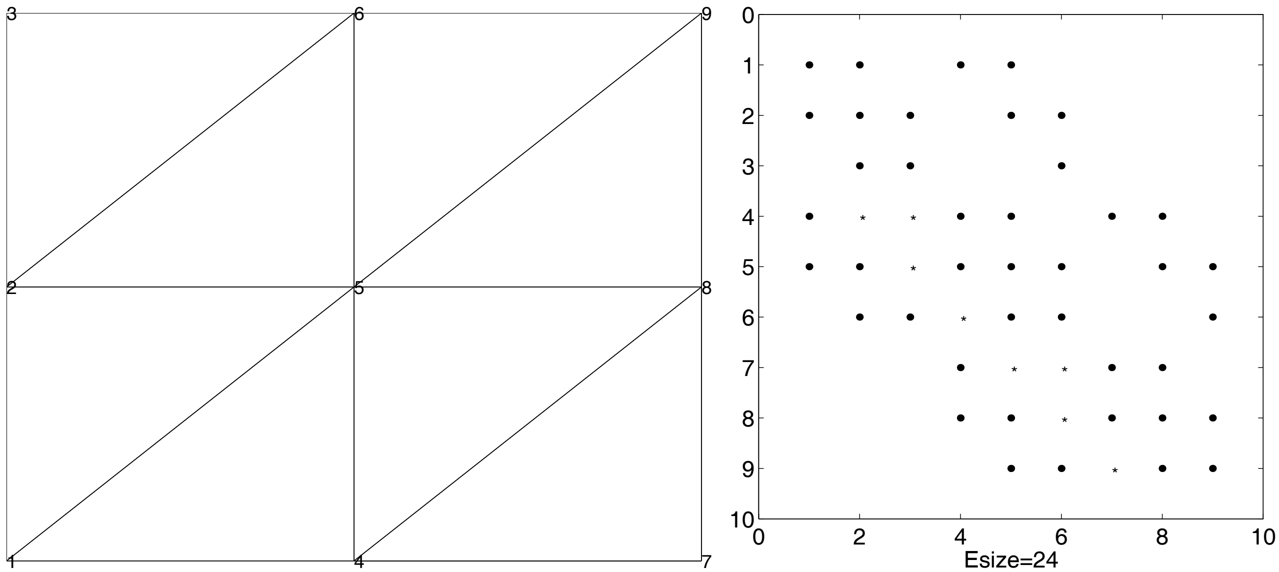

FIG. 2.1. *An ordering of 7-point grid and the corresponding matrix. The lower triangle of the envelope is indicated by marking zeros within it by asterisks.*

i	1	2	3	4	5	6	7	8	9
r_i	0	1	1	3	4	4	3	4	4
c_i	3	4	3	4	4	3	2	1	0

TABLE 2.1
Row-widths and column-widths of the matrix in Figure 1.

the work bound is likely to be intractable as well. So one has to settle for heuristic orderings to reduce these quantities.

It is helpful to consider a "column-oriented" expression for the envelope size for obtaining a lower bound on this quantity in Section 3. The *width* of a column j of A is the number of row indices in the jth column of the envelope of A. In other words,

$$c_j(A) = |\{k : k > j, \text{and } \exists \ell \leq j \ni a_{k\ell} \neq 0\}|.$$

(This is also called the jth *front-width.*) It is then easily seen that the envelope size is

$$\text{Esize}(A) = \sum_{j=1}^{n} c_j. \tag{2.1}$$

The work in an envelope factorization scheme is given by

$$\text{Ework}(A) = (1/2) \sum_{j=1}^{n} c_j^2, \tag{2.2}$$

where we have ignored the linear term in c_j. The column-widths of the matrix in Figure 2.1 are given in Table 2.1. These concepts and their inter-relationships are described by Liu and Sherman [29], and are also discussed in the books [5, 15].

The envelope parameters can also be defined with respect to the adjacency graph $G = (V, E)$ of A. Denote $\mathrm{nbr}(v) = \{v\} \cup \mathrm{adj}(v)$. In terms of the graph G and an ordering α of its vertices, we can define

$$r(v, \alpha) = \max\{\alpha(v) - \alpha(w) : w \in \mathrm{nbr}(v), \alpha(w) \leq \alpha(v)\}.$$

Hence we can write the envelope size and work associated with an ordering α as

$$\begin{aligned}
\mathrm{Esize}(G, \alpha) &= \sum_{v \in V} r(v, \alpha) = \sum_{v \in V} \max\{\alpha(v) - \alpha(w) : w \in \mathrm{nbr}(v), \alpha(w) \leq \alpha(v)\}, \\
\mathrm{Wbound}(G, \alpha) &= \sum_{v \in V} r(v, \alpha)^2 = \sum_{v \in V} \max\{(\alpha(v) - \alpha(w))^2 : w \in \mathrm{nbr}(v), \alpha(w) \leq \alpha(v)\}.
\end{aligned}$$

The goal is to choose a vertex ordering $\alpha : V \mapsto \{1, \ldots, n\}$ to minimize one of the parameters described above. We denote by $\mathrm{Esize}_{\min}(G)$ ($\mathrm{Wbound}_{\min}(G)$) the minimum value of $\mathrm{Esize}(G, \alpha)$ ($\mathrm{Wbound}(G, \alpha)$) over all orderings α. The reader can compute the envelope size of the numbered graph in Figure 2.1, using the definition given in this paragraph, to verify that $\mathrm{Esize}(G) = 24$.

The jth front-width has an especially nice interpretation if we consider the adjacency graph $G = (V, E)$ of A. Let the vertex corresponding to a column j of A be numbered v_j so that $V = \{v_1, \ldots, v_n\}$, and define $V_j = \{v_1, \ldots, v_j\}$. Denote $\mathrm{adj}(X) = (\cup_{v \in X} \mathrm{adj}(v)) \setminus X$, for a subset of vertices X. Then $c_j(A) = |\mathrm{adj}(V_j)|$.

To illustrate the dependence of the envelope size on the ordering, we include in Figure 2.2 an ordering that leads to a smaller envelope size for the 7-point grid. Again, a '$\bullet$' indicates a nonzero element, and a '$*$' indicates a zero element that belongs to the lower triangle of the envelope in the matrix. This ordering by 'diagonals' yields the optimal envelope size for the 7-point grid [27].

2.2. 1- and 2-sum problems. It will be helpful to consider quantities related to the envelope size and envelope work, the 1-sum and the 2-sum.

For real $1 \leq p < \infty$, we define the p-sum to be

$$\sigma_p^p(A) = \sum_{i=1}^{n} \sum_{j \in \mathrm{row}(i)} (i - j)^p.$$

Minimizing the 1-sum ($p = 1$) is the *optimal linear arrangement problem*, and the limiting case $p = \infty$ corresponds to the minimum *bandwidth problem*; both these are well-known NP-complete problems [13]. We show in the Section 2.3 that minimizing the 2-sum is NP-complete as well.

We write the envelope size and 1-sum, and the envelope work and the 2-sum, in a way that shows their relationships:

$$\mathrm{Esize}(A) = \sum_{i=1}^{n} \max_{j \in \mathrm{row}(i)} (i - j), \tag{2.3}$$

$$\sigma_1(A) = \sum_{i=1}^{n} \sum_{j \in \mathrm{row}(i)} (i - j); \tag{2.4}$$

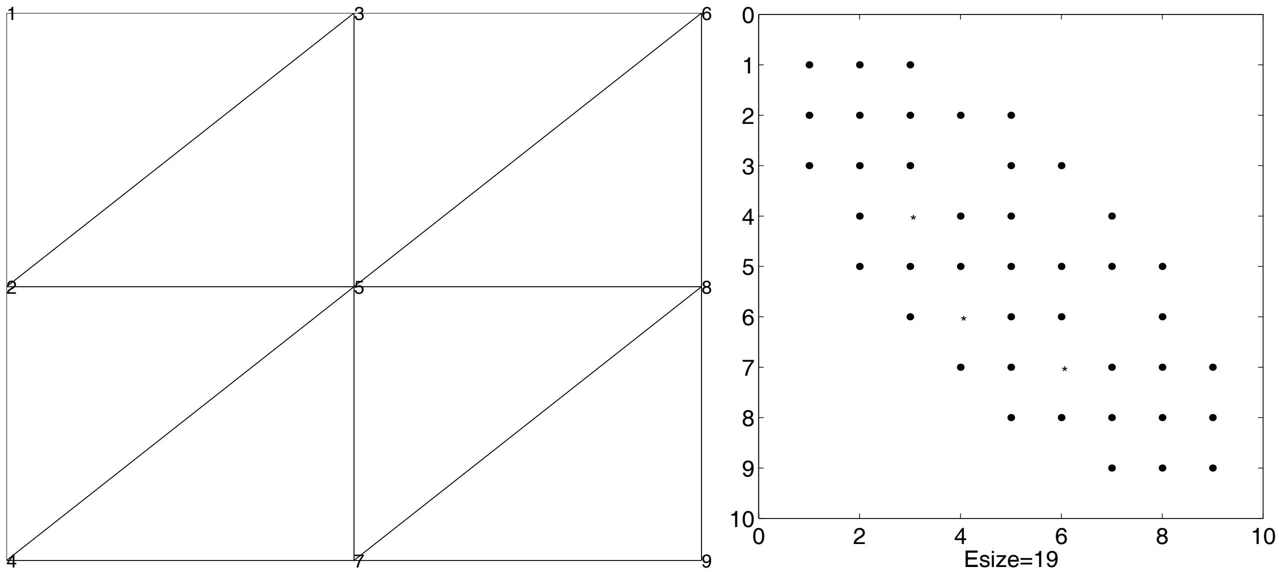

FIG. 2.2. *Another ordering of a 7-point grid and the corresponding matrix. Again the lower triangle of the envelope is indicated by marking the zeros within it by asterisks.*

$$\text{Wbound}(A) = \sum_{i=1}^{n} \max_{j \in \text{row}(i)} (i-j)^2, \tag{2.5}$$

$$\sigma_2^2(A) = \sum_{i=1}^{n} \sum_{j \in \text{row}(i)} (i-j)^2. \tag{2.6}$$

The parameters $\sigma_{1,\min}(A)$ and $\sigma^2_{2,\min}(A)$ are the minimum values of these parameters over all symmetric permutations P^TAP of A.

We now consider the relationships between bounds on the envelope size and the 1-sum, and between the upper bound on the envelope work and the 2-sum. Let Δ denote the maximum number of offdiagonal nonzeros in a row of A. (This is the maximum vertex degree in the adjacency graph of A.)

THEOREM 2.1. *The minimum values of the envelope size, envelope work in the Cholesky factorization,* 1*-sum, and* 2*-sum of a symmetric matrix* A *are related by the following inequalities:*

$$\text{Esize}_{\min}(A) \leq \sigma_{1,\min}(A) \leq \Delta \text{Esize}_{\min}(A); \tag{2.7}$$

$$\text{Wbound}_{\min}(A) \leq \sigma^2_{2,\min}(A) \leq \Delta \text{Wbound}_{\min}(A); \tag{2.8}$$

$$\sigma_{2,min}(A) \leq \sigma_{1,\min}(A) \leq \sqrt{|E|}\, \sigma_{2,min}(A). \tag{2.9}$$

Proof. We begin by proving (2.8). Our strategy will be to first prove the inequalities

$$\text{Wbound}(A) \leq \sigma_2^2(A) \leq \Delta \text{Wbound}(A),$$

and then to obtain the required result by considering two different permutations of A.

The bound $\mathrm{Wbound}(A) \le \sigma_2^2(A)$ is immediate from equations (2.5) and (2.6). If the inner sum in the latter equation is bounded from above by

$$\Delta \max_{j \in row(i)} (i-j)^2,$$

then we get $\Delta\mathrm{Wbound}(A)$ as an upper bound on the 2-sum.

Now let X_1 be a permutation matrix such that $\widetilde{A_1} \equiv X_1^T A X_1$, and $\mathrm{Wbound}(\widetilde{A_1}) = \mathrm{Wbound}_{\min}(A)$. Then we have

$$\sigma_{2,\min}^2(A) \le \sigma_2^2(\widetilde{A_1}) \le \Delta\mathrm{Wbound}(\widetilde{A_1}) = \Delta\mathrm{Wbound}_{\min}(A).$$

Further, let X_2 be a permutation matrix such that $\widetilde{A_2} \equiv X_2^T A X_2$, and $\sigma_2^2(\widetilde{A_2}) = \sigma_{2,\min}^2(A)$. Again, we have

$$\mathrm{Wbound}_{\min}(A) \le \mathrm{Wbound}(\widetilde{A_2}) \le \sigma_2^2(\widetilde{A_2}) = \sigma_{2,\min}^2(A).$$

We obtain the result by putting the last two inequalities together.

We omit the proof of (2.7) since it can be obtained by a similar argument, and proceed to prove (2.9). The first inequality $\sigma_2(A) \le \sigma_1(A)$ holds since the p-norm of any real vector is a decreasing function of p. The second inequality is also standard, since it bounds the 1-norm of a vector by means of its 2-norm. This result was obtained earlier by Juvan and Mohar [24]; we include its proof for completeness. Applying the Cauchy-Schwarz inequality to $\sigma_1^2(A)$ we have

$$\begin{aligned} &\left(\sum_{i=1}^{n} \sum_{j \in \mathrm{row}(i)} (i-j) \right)^2 \\ &\le \left(\sum_{i=1}^{n} \sum_{j \in \mathrm{row}(i)} 1 \right) \left(\sum_{i=1}^{n} \sum_{j \in \mathrm{row}(i)} (i-j)^2 \right) = |E| \sigma_2^2(A). \end{aligned}$$

We obtain the result by considering two orderings that achieve the minimum 1- and 2-sums. □

2.3. Complexity of the 2-sum problem. We proceed to show that minimizing the 2-sum is NP-complete. In Section 8 we show that the spectral algorithm computes a 2-sum within a factor of two for the finite element problems in our test collection. This proof shows that despite the near-optimal solutions obtained by the spectral algorithm on this test set, it is unlikely that a polynomial time algorithm can be designed for computing the minimum 2-sum.

Readers who are willing to accept the complexity of this problem without proof should skip this section; we recommend that everyone do so on a first reading.

Given a graph $G = (V, E)$ on n vertices, MINTWOSUM is the problem of deciding if there exists a numbering of its vertices $\alpha : V \mapsto \{1, \ldots, n\}$ such that $\sum_{(u,v) \in E} (\alpha(u) - \alpha(v))^2 \le k$, for a given positive integer k. This is the decision version of the problem of minimizing the 2-sum of G.

THEOREM 2.2. *MINTWOSUM is NP-complete.*

Remark. This proof follows the framework for the NP-completeness of the 1-sum problem in Even [8] (Section 10.7); but the details are substantially different.

Proof. The theorem will follow if we show that MAXTWOSUM, the problem of deciding whether a graph G' on n vertices has a vertex numbering with 2-sum *greater than or equal to* a given positive integer k', is NP-complete. For, the 2-sum of G' under some ordering is at least k' if and only if the 2-sum of the complement of G' under the same ordering is at most $p(n) - k'$, where $p(n) = \sum_{j=1}^{n} \sum_{i=1}^{j-1} (j-i)^2 = n^4/12 + \Theta(n^3)$ is the 2-sum of the complete graph.

We show that MAXTWOSUM is NP-complete by a reduction from MAXCUT, the problem of deciding whether a given graph $G = (V, E)$ has a partition of its vertices into two sets $\{S, V \setminus S\}$ such that $|\delta(S, V \setminus S)|$, the number of edges joining S and $V \setminus S$, is at least a given positive integer k. From the graph G we construct a graph $G' = (V' \equiv V \cup \{x_1, \ldots, x_{n^4}\}, E' \equiv E)$ by adding n^4 isolated vertices to V and no edges to E. We claim that G has a cut of size at least k if and only if G' has a 2-sum at least $k' \equiv k \cdot n^8$.

If G has a cut $(S, V \setminus S)$ of size at least k, define an ordering α' of G' by interposing the n^4 isolated vertices between S and $V \setminus S$: number the vertices in S first, the isolated vertices next, and the vertices in $V \setminus S$ last, where the ordering among the vertices in each set S and $V \setminus S$ is arbitrary. Every edge belonging to the cut contributes at least n^8 to the 2-sum, and hence its value is at least $k \cdot n^8$.

The converse is a little more involved.

Suppose that G' has an ordering $\alpha' : V' \mapsto \{1, 2, \ldots, n + n^4\}$ with 2-sum greater than or equal to $k \cdot n^8$. The ordering α' of G' induces a natural ordering $\alpha : V \mapsto \{1, \ldots, n\}$ of G, if we ignore the isolated vertices and maintain the relative ordering of the vertices in V. For each $1 \le i \le n$, define the ordered set $S_i = \{v \in V : \alpha(v) \le i\}$. Then each pair $(S_i, V \setminus S_i)$ is a cut in G. Further, each such cut in G induces a cut $(S_i', V' \setminus S_i')$ in the larger graph G' as follows: The vertex set S_i' is formed by augmenting S_i with the isolated vertices numbered lower than the highest numbered (non-isolated) vertex in S_i (with respect to the ordering α').

We now choose a cut $(S', V' \setminus S')$ that maximizes the "1-sum over the cut edges"

$$\sum_{\substack{v \in S', w \in V' \setminus S' \\ (v,w) \in E',}} |\alpha'(v) - \alpha'(w)|,$$

from among the n cuts $(S_i', V' \setminus S_i')$. By means of this cut and the ordering α', we define a new ordering β' by moving the isolated vertices in the ordered set S' to the highest numbers in that set, and by moving the isolated vertices in $V' \setminus S'$ to the lowest numbers in that set, and preserving the relative ordering of the other vertices. The effect is to interpose the isolated vertices in "between" the two sets of the cut.

Claim. The 2-sum of the graph G' under the ordering β' is greater than that under α'.

To prove the claim, we examine what happens when an isolated vertex x belonging to S' is moved to the higher end of that ordered set.

Define three sets A', B', C' as follows: The set A' (B') is the set of vertices in S' numbered lower (higher) than x in the ordering α', and $C' \equiv V' \setminus S'$. Also, let E_1 denote the edges joining A' and B', E_2 denote edges joining B' and C', and E_3 denote those joining A' and C'.

Denote the contribution, with respect to the ordering α', of an edge $e_k \in E_1$ to the 1-sum by a_k, and that of an edge $e_l \in E_2$ by b_l. Then the change in the 2-sum due to moving x is

$$\begin{aligned} & \sum_{E_2}(b_l+1)^2 - b_l^2 \ + \ \sum_{E_1}(a_k-1)^2 - a_k^2 \\ = \ & |E_1| + |E_2| + \sum_{E_2} 2b_l - \sum_{E_1} 2a_k. \end{aligned}$$

The third term on the right-hand-side is the contribution to the 1-sum made by the edges E_2 in the cut $(A' \cup B', C') \equiv (S', V' \setminus S')$, while the fourth term is the contribution made by the edges E_1 in the cut $(A', B' \cup C')$. By the choice of the cut $(S', V' \setminus S')$, we find that the difference is positive, and hence that the 2-sum has increased in the new ordering obtained from α' by moving the vertex x.

We now show that after moving the vertex x, $(A' \cup B', C')$ continues to be a cut that maximizes the 1-sum over the cut edges among all cuts $(S_i', V' \setminus S_i')$ *with respect to the new ordering*. For this cut, the 1-sum over cut edges has increased by $|E_2|$ because the number of each vertex in B has decreased by one in the new ordering. Among cuts with one set equal to an ordered subset of A', the 1-sum over cut edges can only decrease when x is moved, since the set B' moves closer to A', and C' does not move at all relative to A'. Now consider cuts of the form $(A' \cup B_1', B_2' \cup C')$, with B_1' an ordered subset of B', and $B_1' \cup B_2' = B'$. The cut edges now join A' to $B_2' \cup C'$, and B_1' to $B_2' \cup C'$. The edges joining A' to B_2' contribute a smaller value to the 1-sum in the new ordering relative to α', while the edges joining A' to C' contribute the same to the 1-sum in both cuts $A' \cup B', C')$ and $(A' \cup B_1', B_2' \cup C')$ under the new ordering. The edges joining B_1' and B_2' do not change their contribution to the 1-sum in the new ordering. The edges that join B_1' and C' form a subset of the edges that join B' and C', and hence the contribution of the former to the 1-sum is no larger than the contribution of the latter set in the new ordering. This shows that the cut $(A' \cup B', C')$ continues to have a 1-sum over the cut edges larger than or equal to that of any cut $(A' \cup B_1', B_2' \cup C')$. Finally, any cut that includes A', B', and an ordered subset C_1' of C' can be shown by similar reasoning to not have a larger 1-sum than $(S', V' \setminus S')$.

The reasoning in the previous paragraph permits us to move the isolated vertices in S' one by one to the higher end of that set without decreasing the 2-sum while simultaneously preserving the condition that the cut $(S', V' \setminus S')$ has the maximum value of the 1-sum over the cut edges. The argument that we can move the isolated vertices in $V' \setminus S'$ to the beginning of that ordered set follows from symmetry since both the 2-sum and the 1-sum are unchanged when we reverse an ordering. Hence by inducting over the number of isolated vertices moved, the ordering β' has a 2-sum at least as large as the ordering α'. This completes the proof of the claim.

The rest of the proof involves computing an upper bound on the 2-sum of the graph G' under the ordering β' to show that since G' has 2-sum greater than k', the graph G has a cut of size at least k.

Let $\delta \equiv |(S', V' \setminus S')|$. The cut edges contribute at most $\delta \cdot (n^4 + n)^2$ to the upper bound on the 2-sum; the uncut edges contribute at most the 2-sum of a complete graph on

n vertices. The latter is $p(n) \equiv n^4/12 + \Theta(n^3)$. Thus we have, keeping only leading terms,

$$\begin{aligned} & \delta(n^4+n)^2 + (2\delta + (1/12))n^4 \geq kn^8 \\ \Rightarrow \quad & \delta + (2\delta)/n^3 + (1/12)/n^4 \geq k. \end{aligned}$$

The second term on the left hand side is less than 1 for $n > 2$ since the number of cut edges δ is at most $n^2/2$; the third term is less than one for all n. The sum of these two terms is less than 1 for $n > 2$. Hence we conclude that the graph G has a cut with at least k edges. This completes the proof of the theorem. $\square$

3. Bounds for envelope size. In this section we present lower bounds for the minimum envelope size and the minimum work involved in an envelope-Cholesky factorization in terms of the second Laplacian eigenvalue. We will require some background on the Laplacian matrix.

3.1. The Laplacian matrix. The Laplacian matrix $Q(G)$ of a graph G is the $n \times n$ matrix $D - M$, where D is the diagonal degree matrix and M is the adjacency matrix of G. If G is the adjacency graph of a symmetric matrix A, then we could define the Laplacian matrix Q directly from A:

$$q_{ij} = \begin{cases} -1 & \text{if } i \neq j \text{ and } \; a_{ij} \neq 0, \\ 0 & \text{if } i \neq j \text{ and } \; a_{ij} = 0, \\ \sum_{\substack{j=1 \\ j \neq i}}^{n} |q_{ij}| & \text{if } i = j. \end{cases}$$

Note that

$$\begin{aligned} \underline{x}^T Q \underline{x} &= \underline{x}^T D \underline{x} - \underline{x}^T M \underline{x} \\ &= \sum_{\substack{j \leq i \\ a_{ij} \neq 0}} (x_i - x_j)^2. \end{aligned} \tag{3.1}$$

The eigenvalues of $Q(G)$ are the *Laplacian eigenvalues* of G, and we list them as $\lambda_1(Q) \leq \lambda_2(Q) \leq \ldots \leq \lambda_n(Q)$. An eigenvector corresponding to $\lambda_k(Q)$ will be denoted by $\underline{x}_k$, and will be called a kth eigenvector of Q. It is well-known that Q is a singular M-matrix, and hence its eigenvalues are nonnegative. Thus $\lambda_1(Q) = 0$, and the corresponding eigenvector is any nonzero constant vector $\underline{c}$. If G is connected, then Q is irreducible, and then $\lambda_2(Q) > 0$; the smallest nonzero eigenvalues and the corresponding eigenvectors have important properties that make them useful in the solution of various partitioning and ordering problems. These properties were first investigated by Fiedler [9, 10]; as discussed in Section 1, more recently several authors have studied their application to such problems.

3.2. Laplacian bounds for envelope parameters. It will be helpful to work with the "column-oriented" definition of the envelope size. Let the vertex corresponding to a column j of A be numbered v_j in the adjacency graph so that $V = \{v_1, \ldots, v_n\}$, and let $V_j = \{v_1, \ldots, v_j\}$. Recall that the *column width* of a vertex v_j is $c_j = |\text{adj}(V_j)|$, and that the envelope size of G (or A) is

$$\text{Esize}(G) = \sum_{j=1}^{n} c_j.$$

Recall also that Δ denotes the maximum degree of a vertex. Given a set of vertices S, we denote by $\delta(S)$ the set of edges with one endpoint in S and the other in $V \setminus S$.

We make use of the following elementary result, where the lower bound is due to Alon and Milman [1] and the upper bound is due to Juvan and Mohar [24].

LEMMA 3.1. *Let $S \subset V$ be a subset of the vertices of a graph G. Then*

$$\lambda_2(Q)\frac{|S||V \setminus S|}{n} \leq |\delta(S)| \leq \lambda_n(Q)\frac{|S||V \setminus S|}{n}. \quad \square$$

THEOREM 3.2. *The envelope size of a symmetric matrix A can be bounded in terms of the eigenvalues of the associated Laplacian matrix as*

$$\frac{\lambda_2(Q)}{6\Delta}(n^2 - 1) \leq \mathrm{Esize}(A) \leq \frac{\lambda_n(Q)}{6}(n^2 - 1).$$

Proof. From Lemma 3.1,

$$|\delta(V_j)| \geq \frac{\lambda_2(Q)}{n} j(n - j).$$

Now $c_j(A) = |\mathrm{adj}(V_j)| \geq |\delta(V_j)|/\Delta$; substituting the lower bound for $|\delta(V_j)|$, and summing this latter expression over all j, we obtain the lower bound on the envelope size.

The upper bound is obtained by using the inequality $c_j(A) \leq |\delta(V_j)|$ with the upper bound in Lemma 3.1. $\square$

A lower bound on the work in an envelope-Cholesky factorization can be obtained from the lower bound on the envelope size.

THEOREM 3.3. *A lower bound on the work in the envelope-Cholesky factorization of a symmetric positive definite matrix A is*

$$\mathrm{Ework}(A) \geq \frac{\mathrm{Esize}(A)^2}{2n}.$$

Proof. The proof follows from Equations 2.1 and 2.2, by an application of the Cauchy-Schwarz inequality. We omit the details. $\square$

Cuthill and McKee [3] proposed one of the earliest ordering algorithms for reducing the envelope size of a sparse matrix. George [14] discovered that reversing this ordering leads to a significant reduction in envelope size and work. The envelope parameters obtained from the reverse-Cuthill-McKee (RCM) ordering are never larger than those obtained from CM [29]. The RCM ordering has become one of the most popular envelope size reducing orderings. However, we do not know of any published quantitative results on the improvement that may be expected by reversing an ordering, and here we present the first such result. For degree-bounded finite element meshes, no asymptotic improvement is possible; the parameters are improved only by a constant factor. Of course, in practice, a reduction by a constant factor could be quite significant.

THEOREM 3.4. *Reversing the ordering of a sparse symmetric matrix A can change (improve or impair) the envelope size by at most a factor Δ, and the envelope work by at most Δ^2.*

Proof. Let v_j denote the vertex in the adjacency graph corresponding to the jth column of A (in the original ordering) so that the jth column width $c_j(A) = |\mathrm{adj}(V_j)|$, where $V_j = \{v_1, \ldots, v_j\}$. Let $\widetilde{A}$ denote the permuted matrix obtained by reversing the column and row ordering of A. We have the inequality

$$c_j(A) = |\mathrm{adj}(V_j)| \le |\delta(V_j)| \le \Delta |\mathrm{adj}(V \setminus V_j)| = \Delta c_{n-j}(\widetilde{A}).$$

Since $\mathrm{Esize}(A) = \sum_{j=1}^{n} c_j(A)$, summing this inequality over j from one to n, we obtain $\mathrm{Esize}(A) \le \Delta \mathrm{Esize}(\widetilde{A})$. By symmetry, the inequality $\mathrm{Esize}(\widetilde{A}) \le \Delta \mathrm{Esize}(A)$ holds as well.

The inequality on the envelope work follows by a similar argument from the equation $\mathrm{Ework}(A) = (1/2) \sum_{j=1}^{n} c_j^2$. $\square$

4. Quadratic assignment formulation of 2- and 1-sum problems. We formulate the 2- and 1-sum problems as quadratic assignment problems in this section.

4.1. The 2-sum problem. Let the vector $\underline{p} = \begin{pmatrix} 1 & 2 & \cdots & n \end{pmatrix}^T$, and let $\underline{\alpha}$ be a permutation vector, i.e., a vector whose components form a permutation of 1, ..., n. We may write $\underline{\alpha} = X\underline{p}$, where X is a permutation matrix with elements

$$x_{ij} = \begin{cases} 1, & \text{if } j = \alpha(i) \\ 0, & \text{otherwise} \end{cases} .$$

It is easily verified that the $(\alpha(i), \alpha(j))$ element of the permuted matrix $X^T A X$ is the element a_{ij} of the unpermuted matrix A. Let $B = \underline{p}\,\underline{p}^T$; then $b_{ij} = ij$. We denote the set of all permutation vectors with n components by S_n.

We write the 2-sum as a quadratic form involving the Laplacian matrix Q.

$$\begin{aligned}
\sigma^2_{2,\min}(A) &= \min_X \sigma_2^2(X^T A X) \\
&= \min_{\underline{\alpha} \in S_n} \sum_{\substack{\alpha(j) \le \alpha(i) \\ a_{\alpha(i),\alpha(j)} \ne 0}} (\alpha(i) - \alpha(j))^2 \\
&= \min_{\underline{\alpha} \in S_n} \underline{\alpha}^T Q \underline{\alpha} \\
&= \min_{\underline{\alpha} \in S_n} \sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij}\, \alpha(i)\alpha(j).
\end{aligned}$$

The transformation from the second to the third line makes use of (3.1).

This quadratic form can be expressed as a quadratic assignment problem by substituting $b_{\alpha(i),\alpha(j)} = \alpha(i)\alpha(j)$:

$$\min_{\underline{\alpha} \in S_n} \underline{\alpha}^T Q \underline{\alpha} \quad = \quad \min_{\underline{\alpha} \in S_n} \sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij}\, b_{\alpha(i)\alpha(j)}.$$

There is also a trace formulation of the QAP in which the variables are the elements of the permutation matrix X. We obtain this formulation by substituting $X\underline{p}$ for $\underline{\alpha}$. Thus

$$\min_{\underline{\alpha}\in S_n} \underline{\alpha}^T Q \underline{\alpha} \quad = \quad \min_X \underline{p}^T X^T Q X \underline{p}.$$

We may consider the last scalar expression as the trace of a 1×1 matrix, and then use the identity $\operatorname{tr} MN = \operatorname{tr} NM$ to rewrite the right-hand-side of the last displayed equation as

$$\min_X \operatorname{tr} QX\underline{p}\,\underline{p}^T X^T \equiv \min_X \operatorname{tr} QXBX^T.$$

This is a quadratic assignment problem since it is a quadratic in the unknowns x_{ij}, which are the elements of the permutation matrix X. The fact that B is a rank-one matrix leads to great simplifications and savings in the computation of good lower bounds for the 2-sum problem.

4.2. The 1-sum problem. Let M be the adjacency matrix of a given symmetric matrix A and let S denote a 'distance matrix' with elements $s_{ij} = |i-j|$, both of order n. Then

$$\begin{aligned}
\sigma_{1,\min}(A) &= \min_X \sigma_1(X^T AX) \\
&= \min_{\underline{\alpha}\in S_n} \sum_{\substack{\alpha(j)\le\alpha(i) \\ m_{\alpha(i),\alpha(j)}\neq 0}} \alpha(i)-\alpha(j) \\
&= (1/2) \min_{\underline{\alpha}\in S_n} \sum_{i=1}^n \sum_{j=1}^n m_{ij}\; s_{\alpha(i),\alpha(j)} \\
&= (1/2) \min \operatorname{tr} MXSX^T.
\end{aligned}$$

Unlike the 2-sum, the matrices involved in the QAP formulation of the 1-sum are both of rank n. Hence the bounds we obtain for this problem by this approach are considerably more involved, and will not be considered here.

5. Eigenvalue bounds for the 2-sum problem.

5.1. Orthogonal bounds. A technique for obtaining lower (upper) bounds for the QAP

$$\min_X \operatorname{tr} QXBX^T, \quad X \text{ is a permutation matrix,}$$

is to relax the requirement that the minimum (maximum) be attained over the class of permutation matrices. Let $\underline{u} = (1/\sqrt{n}) \begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix}$ denote the normalized n-vector of all ones. A matrix X of order n is a permutation matrix if and only if it satisfies the following three constraints:

$$X\underline{u} = \underline{u}, \quad X^T\underline{u} = \underline{u}; \tag{5.1}$$

$$X^T X = I_n; \tag{5.2}$$

$$x_{ij} \ge 0, \; i,j = 1,\dots,n. \tag{5.3}$$

The first of these, the *stochasticity constraint*, expresses the fact that each row sum or column sum of a permutation matrix is one; the second states that a permutation matrix is orthogonal; and the third that its elements are non-negative. The simplest bounds for a QAP are obtained when we relax both the stochasticity and non-negativity constraints, and insist only that X be orthonormal. The following result is from [11]; see also [12].

THEOREM 5.1. *Let the eigenvalues of a matrix be ordered*

$$\lambda_1(\cdot) \leq \lambda_2(\cdot) \cdots \leq \lambda_n(\cdot)\,.$$

Then, as X varies over the set of orthogonal matrices, the following upper and lower bounds hold:

$$\sum_{i=1}^{n} \lambda_i(Q)\lambda_{n+1-i}(B) \leq \operatorname{tr} QXBX^T \leq \sum_{i=1}^{n} \lambda_i(Q)\lambda_i(B). \quad \Box$$

The Laplacian matrix Q has $\lambda_1(Q) = 0$; also $\lambda_i(B) = 0$, for $i = 1, \ldots, n-1$, and $\lambda_n(B) = \underline{p}^T \underline{p} = (1/6)n(n+1)(2n+1)$. Hence the lower bound in the theorem above is zero, and the upper bound is $(1/6)\lambda_n(Q)n(n+1)(2n+1)$.

5.2. Projection bounds. Stronger bounds can be obtained by a projection technique described by Hadley, Rendl, and Wolkowicz [19]. The idea here is to satisfy the stochasticity constraints in addition to the orthonormality constraints, and relax only the non-negativity constraints. This technique involves projecting a permutation matrix X into a subspace orthogonal to the stochasticity constraints (5.1) by means of an eigenprojection.

Let the $n \times n-1$ matrix V be an orthonormal basis for the orthogonal complement of $\underline{u}$. By the choice of V, it satisfies two properties: $V^T\underline{u} = \underline{0}$, and $P = \begin{pmatrix} \underline{u} & V \end{pmatrix}$ is an orthonormal matrix of order n.

Observe that

$$P^TXP = \begin{pmatrix} \underline{u}^T \\ V^T \end{pmatrix} X \begin{pmatrix} \underline{u} & V \end{pmatrix} = \begin{pmatrix} \underline{u}^TX\underline{u} & \underline{u}^TXV \\ V^TX\underline{u} & V^TXV \end{pmatrix} = \begin{pmatrix} 1 & \underline{0}^T \\ \underline{0} & Y \end{pmatrix},$$

where $Y \equiv V^TXV$.

This suggests that we take

$$\begin{aligned} X &= P \begin{pmatrix} 1 & \underline{0}^T \\ \underline{0} & Y \end{pmatrix} P^T \\ &= \underline{u}\,\underline{u}^T + VYV^T. \end{aligned} \tag{5.4}$$

Note that with this choice, the stochasticity constraints $X\underline{u} = \underline{u}$ and $X^T\underline{u} = \underline{u}$ are satisfied. Furthermore, if X is an orthonormal matrix of order n satisfying $X\underline{u} = \underline{u}$, then

$$P^TXP = \begin{pmatrix} 1 & \underline{0}^T \\ \underline{0} & Y \end{pmatrix}$$

is orthonormal, and this implies that Y is an orthonormal matrix of order $n-1$. Conversely, if Y is orthonormal of order $n-1$, then the matrix X obtained by the construction above is orthonormal of order n. The non-negativity constraint $X \geq 0$ becomes, from (5.4), $VYV^T \geq -\underline{u}\,\underline{u}^T$. These facts will enable us to express the original QAP in terms of a projected QAP in the matrix of variables Y.

To obtain the projected QAP, we substitute the representation of X from (5.4) into the objective function $\mathrm{tr}\, QXBX^T$. Since $Q\underline{u} = \underline{0}$ by the construction of the Laplacian, terms of the form $Q\underline{u}\,\underline{u}^T \cdots$ vanish. Further,

$$\mathrm{tr}\, QVYV^T B\underline{u}\,\underline{u}^T = \mathrm{tr}\, \underline{u}^T QVYV^T B\underline{u},$$

where we use the identity $\mathrm{tr}\, MN = \mathrm{tr}\, NM$ for an $n \times k$ matrix M and a $k \times n$ matrix N. Again this term is zero since $\underline{u}^T Q = \underline{0}^T$. Hence the only nonzero term in the objective function is

$$\begin{aligned}
&\mathrm{tr}\, Q\; VYV^T\; B\; VY^T V^T \\
&\quad = \ \mathrm{tr}\, (V^T QV)\, Y\, (V^T BV)\, Y^T \\
&\quad = \ \mathrm{tr}\, \widehat{Q} Y \widehat{B} Y^T,
\end{aligned}$$

where $\widehat{M} = V^T MV$ is a projection of a matrix M.

We have obtained the projected QAP in terms of the matrix Y of order $n-1$, where the constraint that X be a permutation matrix now imposes the constraints that Y is orthonormal and that $VYV^T \geq -\underline{u}\,\underline{u}^T$. We obtain lower and upper bounds in terms of the eigenvalues of the matrices $\widehat{Q}$ and $\widehat{B}$ by relaxing the non-negativity constraint again.

Theorem 5.2. *The following upper and lower bounds hold for the 2-sum problem:*

$$(1/12)\lambda_2(Q)(n-1)n(n+1) \leq \sigma_2^2(A) \leq (1/12)\lambda_n(Q)(n-1)n(n+1).$$

Proof. If we apply the orthogonal bounds to the projected QAP, we get

$$\sum_{i=1}^{n-1} \lambda_i(\widehat{Q})\lambda_{n-i}(\widehat{B}) \leq \sigma_2^2(A) \leq \sum_{i=1}^{n-1} \lambda_i(\widehat{Q})\lambda_i(\widehat{B}).$$

The vector $\underline{u}$ is the eigenvector of Q corresponding to the zero eigenvalue, and hence eigenvectors corresponding to higher Laplacian eigenvalues are orthogonal to it. Thus any such eigenvector $\underline{x}_j$ can be expressed as $\underline{x}_j = V\underline{r}_j$. Substituting this last equation into the eigenvalue equation $Q\underline{x}_j = \lambda_j(Q)\underline{x}_j$, and pre-multiplying by V^T, we obtain $\widehat{Q}\underline{r}_j = \lambda_j(Q)\underline{r}_j$. Hence for $i = 2, \ldots, n$, we have $\lambda_i(Q) = \lambda_{i-1}(\widehat{Q})$. Also, $\lambda_{n-1}(\widehat{B}) = \underline{p}^T VV^T \underline{p}$, and all other eigenvalues are zero. Hence it remains to compute the largest eigenvalue of $\widehat{B}$.

From the representation $I_n = PP^T = \underline{u}\,\underline{u}^T + VV^T$, we compute

$$\begin{aligned}
&\underline{p}^T VV^T \underline{p} \\
&\quad = \ \underline{p}^T\, \underline{p} - (\underline{p}^T\, \underline{u})\, (\underline{u}^T\, \underline{p}) \\
&\quad = \ (1/6)n(n+1)(2n+1) - (1/4)n(n+1)^2 \ = \ (1/12)(n-1)n(n+1).
\end{aligned}$$

We get the result by substituting these eigenvalues into the bounds for the 2-sum. □

For justifying the spectral algorithm for minimizing the 2-sum, we observe that the lower bound is attained by the matrix

$$X_0 = \underline{u}\,\underline{u}^T + VRS^TV^T, \tag{5.5}$$

where R (S) is a matrix of eigenvectors of $\widehat{Q}$ ($\widehat{B}$), and the eigenvectors correspond to the eigenvalues of $\widehat{Q}$ ($\widehat{B}$) in non-decreasing (non-increasing) order.

The result given above has been obtained by Juvan and Mohar [24] without using a QAP formulation of the 2-sum. We have included this proof for two reasons: First, in the next subsection, we show how the lower bound may be strengthened by diagonal perturbations of the Laplacian. Second, in the following section, we consider the problem of finding a permutation matrix closest to the orthogonal matrix attaining the lower bound.

5.3. Diagonal perturbations. The lower bound for the 2-sum can be further improved by perturbing the Laplacian matrix Q by a diagonal matrix $Diag(\underline{d})$, where $\underline{d}$ is an n-vector, and then using an optimization routine to maximize the smallest eigenvalue of the perturbed matrix.

Choosing the elements of $\underline{d}$ such that its elements sum to zero, i.e., $\underline{u}^T\underline{d} = 0$, simplifies the bounds we obtain, and hence we make this assumption in this subsection. We begin by denoting $Q(d) = Q + Diag(\underline{d})$, and expressing

$$f(X) \equiv \mathrm{tr}\, QXBX^T = \mathrm{tr}\, Q(d)XBX^T - \mathrm{tr}\, Diag(\underline{d})XBX^T.$$

The second term can be written as a linear assignment problem (LAP) since one of the matrices involved is diagonal. Let the permutation vector $\underline{\alpha} = X\underline{p}$, and let $\underline{d}_B$ denote the n-vector formed from the diagonal elements of B.

$$\mathrm{tr}\, Diag(\underline{d})XBX^T \;=\; \sum_{i=1}^{n} d_i b_{\alpha(i),\alpha(i)} \;=\; \mathrm{tr}\, \underline{d}\,\underline{d}_B{}^T X^T.$$

We now proceed, as in the previous subsection, to obtain projected bounds for the quadratic term, and thus for $f(X)$. Note that $Q(d)\underline{u} = (1/\sqrt{n}\,)\underline{d}$ since $Q\underline{u} = \underline{0}$; and $\underline{u}^TQ(d)\underline{u} = 0$ since the elements of $\underline{d}$ sum to zero. We let $B\underline{u} = (1/\sqrt{n}\,)\,\underline{r}(B)$ denote the row-sum of the elements of B.

With notation as in the previous subsection, we substitute $X = \underline{u}\,\underline{u}^T + VYV^T$ in the quadratic term in $f(X)$. The first term $\mathrm{tr}\, Q(d)\underline{u}\,\underline{u}^TB\underline{u}\,\underline{u}^T = \mathrm{tr}\,\underline{u}^TQ(d)\underline{u}\,\underline{u}^TB\underline{u} = 0$. The second and third terms are equal, and their sum can be transformed as follows:

$$\begin{aligned} &2\,\mathrm{tr}\, Q(d)VYV^TB\underline{u}\,\underline{u}^T = 2\,\mathrm{tr}\,\underline{u}^TQ(d)VYV^TB\underline{u} \\ &\quad= \;(2/n)\,\mathrm{tr}\,\underline{d}^TVYV^T\underline{r}(B) \;=\; (2/n)\,\mathrm{tr}\,V^T\underline{r}(B)\,\underline{d}^TVY \\ &\quad= \;(2/n)\,\mathrm{tr}\,Y^TV^T\underline{d}\,\underline{r}(B)^TV \;=\; (2/n)\,\mathrm{tr}\,\underline{d}\,\underline{r}(B)^TVY^TV^T. \end{aligned}$$

Note that this term is linear in the projected variables Y, and we shall find it convenient to express it in terms of X by the substitution $X^T - \underline{u}\,\underline{u}^T = VY^TV^T$. Thus

$$(2/n)\,\mathrm{tr}\,\underline{d}\,\underline{r}(B)^TVY^TV^T \;=\; (2/n)\,\mathrm{tr}\,\underline{d}\,\underline{r}(B)^T(X^T - \underline{u}\,\underline{u}^T) \;=\; (2/n)\,\mathrm{tr}\,\underline{d}\,\underline{r}(B)^TX^T,$$

since the second term is equal to $\operatorname{tr} \underline{u}^T \, \underline{d} \, \underline{r}(B)^T \underline{u}$, which is zero by the choice of $\underline{d}$.

Finally, the fourth term becomes $\operatorname{tr} \widehat{Q}(d) Y \widehat{B} Y^T$, where $\widehat{Q}(d) = V^T Q(d) V$, and as before $\widehat{B} = V^T B V$.

Putting it all together, we obtain

$$f(X) = \operatorname{tr} \widehat{Q}(d) Y \widehat{B} Y^T + \operatorname{tr} \left((2/n) \underline{d} \, \underline{r}(B)^T X^T - \underline{d} \, \underline{d_B}^T X^T \right).$$

Observe that the first term is quadratic in the projected variables Y, and the remaining terms are linear in the original variables X. Our lower bound for the 2-sum shall be obtained by minimizing the quadratic and linear terms separately.

We can simplify the linear assignment problem by noting that $B = \underline{p} \, \underline{p}^T$. Thus $r_{B,i} = i \sum_{j=1}^{n} j = (1/2)n(n+1)i$, and hence $(2/n)\underline{r}(B) = (n+1)\underline{p}$. Further, $\underline{d_B} = sq(\underline{p})$, the vector with ith component equal to i^2. Hence the final expression for the linear assignment problem is

$$\operatorname{tr} \underline{d} \left((n+1)\underline{p}^T - sq(\underline{p})^T \right) X^T.$$

The minimum value of this problem, denoted by $L(\underline{d})$ (the minimum over the permutation matrices X, for a given $\underline{d}$), can be computed by sorting the components of $\underline{d}$ and $\left((n+1)\underline{p} - sq(\underline{p})\right)$.

The eigenvalues of $\widehat{B}$ can be computed as in the previous subsection. We may choose $\underline{d}$ to maximize the lower bound. Thus this discussion leads to the following result.

Theorem 5.3. *The minimum 2-sum of a symmetric matrix A can be bounded as*

$$\sigma_{2,\min}^2(A) \geq \max_{\underline{d}} \left\{ (1/12)\lambda_1(\widehat{Q}(d))(n-1)n(n+1) + L(\underline{d}) \right\},$$

where the components of the vector $\underline{d}$ sum to zero. $\square$

6. Computing an approximate solution from the lower bound. Consider the problem of finding a permutation matrix Z "closest" to an orthogonal matrix X_0 that attains the lower bound in Theorem 5.2. We show in this section that sorting the second Laplacian eigenvector components in non-increasing (also non-decreasing) order yields a permutation matrix that solves a linear approximation to the problem. This justifies the spectral approach for minimizing the 2-sum.

From (5.5), the orthogonal matrix $X_0 = \underline{u} \, \underline{u}^T + V R S^T V^T$, where R (S) is a matrix of eigenvectors of $\widehat{Q}$ ($\widehat{B}$) corresponding to the eigenvalues of $\widehat{Q}$ ($\widehat{B}$) in increasing (decreasing) order. We begin with a preliminary discussion of some properties of the matrix X_0 and the eigenvectors of Q. For $j = 1, \ldots, n-1$, let the jth column of R be denoted by $\underline{r}_j$, and similarly let $\underline{s}_j$ denote the jth column of S. Then $\underline{s}_1 = c V^T \underline{p}$, where c is a normalization constant; for $j = 2, \ldots, n-1$, the vector $\underline{s}_j$ is orthogonal to $V^T \underline{p}$, i.e.,

$$\underline{s}_j^T V^T \underline{p} = 0. \tag{6.1}$$

Recall from the previous section that a second Laplacian eigenvector $\underline{x}_2 = V \underline{r}_1$.

Now we can formulate the "closest" permutation matrix problem more precisely. The minimum 2-sum problem may be written as

$$\min_Z \; \|(Q+\alpha I)^{1/2} Z \underline{p}\|_2{}^2.$$

We have chosen a positive shift α to make the shifted matrix positive definite and hence to obtain a weighted norm by making the square root nonsingular. It can be verified that the shift has no effect on the minimizer since it adds only a constant term to the objective function.

We substitute $Z = X_0 + (Z - X_0)$ and expand the 2-sum about X_0 to obtain

$$\begin{aligned} &\|(Q+\alpha I)^{1/2} Z \underline{p}\|_2{}^2 = \\ (6.2)\quad &\|(Q+\alpha I)^{1/2} X_0\, \underline{p}\|_2{}^2 + 2\,\mathrm{tr}\, \underline{p}^T (Z-X_0)^T (Q+\alpha I) X_0\, \underline{p} + \|(Q+\alpha I)^{1/2}(Z-X_0)\, \underline{p}\|_2{}^2. \end{aligned}$$

The first term on the right-hand-side is a constant since X_0 is a given orthogonal matrix; the third term is a quadratic in the difference $(Z - X_0)$ and hence we neglect it to obtain a linear approximation. It follows that we can choose a permutation matrix Z close to X_0 to approximately minimize the 2-sum by solving

$$(6.3)\qquad \min_Z \mathrm{tr}\, \underline{p}^T Z^T (Q+\alpha I) X_0\, \underline{p} \quad = \quad \min_Z \; \mathrm{tr}\, (Q+\alpha I) X_0 B Z^T.$$

Substituting for X_0 from (5.5) in this linear assignment problem and noting that $Q\underline{u} = \underline{0}$, we find

$$\begin{aligned} &\min_Z \; \mathrm{tr}\,(Q+\alpha I) X_0 B Z^T = \min_Z \; \mathrm{tr}\,(Q+\alpha I)\,(\underline{u}\,\underline{u}^T + VRS^TV^T) B Z^T \\ (6.4)\qquad &= \; \min_Z \; \left(\mathrm{tr}\, QVRS^TV^TBZ^T + \alpha\,\mathrm{tr}\,\underline{u}\,\underline{u}^T B Z^T + \alpha\,\mathrm{tr}\, VRS^TV^TBZ^T\right). \end{aligned}$$

The second term on the right-hand-side is a constant since

$$\mathrm{tr}\,\underline{u}\,\underline{u}^T B Z^T \;=\; \mathrm{tr}\,\underline{u}^T B Z^T \underline{u} \;=\; \mathrm{tr}\,\underline{u}^T B \underline{u} \;=\; (\underline{u}^T\,\underline{p})^2.$$

Here we have substituted $Z^T\underline{u} = \underline{u}$ from (5.1). We proceed to simplify the first term in (6.4), which is

$$\mathrm{tr}\, QVRS^TV^TBZ^T \quad = \quad \mathrm{tr}\, QV \left(\sum_{j=1}^{n-1} \underline{r}_j\, \underline{s}_j{}^T\right) V^T \underline{p}\,\underline{p}^T Z^T.$$

From (6.1) we find that $\underline{s}_j{}^T V^T \underline{p} = 0$, for $j = 2, \ldots, n-1$, and hence *only the first term in the sum survives.* Noting that $\underline{s}_1 = cV^T\underline{p}$, and $V\underline{r}_1 = \underline{x}_2$, this term becomes

$$\mathrm{tr}\, Q\underline{x}_2\,(c\underline{p}^T V)\, V^T \underline{p}\,\underline{p}^T Z^T \quad = \quad c\lambda_2(Q)(\underline{p}^T V V^T \underline{p})\,\mathrm{tr}\,\underline{x}_2\,\underline{p}^T Z^T.$$

The third term in (6.4) can be simplified in like manner, and hence ignoring the constant second term, this equation becomes

$$c(\lambda_2(Q)+\alpha)\,(\underline{p}^T V V^T \underline{p})\,\min_Z \; \mathrm{tr}\,\underline{x}_2\,\underline{p}^T Z^T.$$

Hence we are required to choose a permutation matrix Z to minimize tr $\underline{x}_2\, \underline{p}^T Z^T =$ tr $Z^T \underline{x}_2\, \underline{p}^T$. The solution to this problem is to choose Z to correspond to a permutation of the components of $\underline{x}_2$ in non-increasing order, since the components of the vector $\underline{p}$ are in increasing order. Note that $-\underline{x}_2$ is also an eigenvector of the Laplacian matrix, and since the positive or negative signs of the components are chosen arbitrarily, sorting the eigenvector components into non-decreasing order also gives a permutation matrix Z closest, within a linear approximation, to a different choice for the orthogonal matrix X_0 (see 5.5).

Similar techniques can be used to show that if one is interested in *maximizing* the 2-sum, then a closest permutation matrix to the orthogonal matrix that attains the upper bound in Theorem 5.2 is approximated by sorting the components of the Laplacian eigenvector $\underline{x}_n$ (corresponding to the largest eigenvalue $\lambda_n(Q)$) in non-decreasing (non-increasing) order.

7. Asymptotic behavior of envelope parameters. In this section, we first prove that graphs with good separators have asymptotically small envelope parameters, and next study the asymptotic behavior of the lower bounds on the envelope parameters as a function of the problem size.

7.1. Upper bounds on envelope parameters. Let α, β, and γ be constants such that $(1/2) \leq \alpha, \gamma < 1$, and define $n_0 \equiv (\beta/(1-\alpha))^{1/(1-\gamma)}$. A class of graphs $\mathcal{G}$ has n^γ-separators if every graph G on $n > n_0$ vertices in $\mathcal{G}$ can be partitioned into three sets A, B, S such that no vertex in A is adjacent to any vertex in B, and the number of vertices in the sets are bounded by the relations $|A|, |B| \leq \alpha n$ and $|S| \leq \beta n^\gamma$. If $n \leq n_0$, then we choose the separator S to consist of the entire graph. If $n > n_0$, then by the choice of n_0,

$$\alpha n + \beta n^\gamma = n\left(\alpha + \beta n^{\gamma-1}\right) < n\left(\alpha + \beta n_0^{\gamma-1}\right) = n,$$

and we separate the graph into two parts A and B by means of a separator S. The assumption that γ is at least a half is not a restriction for the classes of graphs that we are interested in here: Planar graphs have $n^{1/2}$-separators, and overlap graphs [30] embedded in $d \geq 2$ dimensions, have $n^{(d-1)/d}$-separators. The latter class includes "well-shaped" finite element graphs in d dimensions, i.e., finite element graphs with elements of bounded aspect ratio.

THEOREM 7.1. *Let $\mathcal{G}$ be a class of graphs that has n^γ-separators and maximum vertex degree bounded by Δ. The minimum envelope size* $\mathrm{Esize}_{\min}(G)$ *of any graph $G \in \mathcal{G}$ on n vertices is $\mathcal{O}(n^{1+\gamma})$.*

Proof. If $n \leq n_0$, then we order the vertices of G arbitrarily. Otherwise, let a separator S separate G into the two sets A and B, where we choose the subset B to have no more vertices than A. We consider a "modified nested dissection" ordering of G that orders the vertices in A first, the vertices in S next, and the vertices in B last. (See the ordering in Figure 2.1, where S corresponds to the set of vertices in the middle column.)

The contribution to the envelope E_S made by the vertices in S is bounded by the product of the maximum row-width of a vertex in S and the number of vertices in S. Thus

$$E_S \leq |S| \cdot |A \cup S| \;\leq\; \beta n^\gamma(\alpha n + \beta n^\gamma) \;=\; \alpha\beta n^{1+\gamma} + \beta^2 n^{2\gamma}.$$

We also consider the contribution made by vertices in B that are adjacent to nodes in S, as a consequence of numbering the nodes in S. There are at most $\Delta|S|$ such vertices in B.

Since these vertices are not adjacent to any vertex in A, the contribution E_B made by them is

$$E_B \leq \Delta|S| \cdot |B \cup S| \ \leq \ \Delta\beta n^\gamma(\alpha n + \beta n^\gamma) \ = \ \Delta\alpha\beta n^{1+\gamma} + \Delta\beta^2 n^{2\gamma}.$$

Let n_1 (n_2) denote the number of vertices in the subset A (B). Adding the contributions from the two sets of nodes in the previous paragraph, we obtain the recurrence relation

$$\begin{aligned} E(n) \ &\leq \ \alpha\beta(1+\Delta)n^{1+\gamma} + \beta^2(1+\Delta)n^{2\gamma} + \max_{n_1,n_2}\left(E(n_1)+E(n_2)\right), \\ &\quad \text{where} \quad n_1, n_2 \leq \alpha n, \quad \text{and } n_1 + n_2 \leq n. \end{aligned} \tag{7.1}$$

We claim that

$$E(n) \leq C_1 n^{1+\gamma} + C_2 n^{2\gamma}\log n, \tag{7.2}$$

for suitable constants C_1 and C_2 to be chosen later. We prove the claim by induction on n.

For $n \leq n_0$, the claim may be satisfied by choosing C_1 to be greater than or equal to $(n_0+1)/2$, since

$$E(n) \leq n(n+1)/2 \leq n(n_0+1)/2 \leq C_1 n^{1+\gamma}.$$

Now consider the case when $n > n_0$. Let the maximum in the recurrence relation (7.1) be attained for $n_1 = an$ and $n_2 = bn \leq (1-a)n$, where $1/2 \leq a \leq \alpha < 1$. Since $n > n_0$, we have $n_1, n_2 < n$; thus the inductive hypothesis can be applied to the subgraphs induced by A and B. Hence we substitute the bound (7.2) into the recurrence relation (7.1) to obtain

$$\begin{aligned} E(n) \ &\leq \ \Big(\alpha\beta(1+\Delta) + C_1(a^{1+\gamma} + (1-a)^{1+\gamma})\Big)\, n^{1+\gamma} \\ &+ \ \Big(\beta^2(1+\Delta) + C_2(a^{2\gamma}\log an + (1-a)^{2\gamma}\log(1-a)n)\Big)\, n^{2\gamma}. \end{aligned}$$

For the claim to be satisfied, this bound must be less than the right-hand-side of the inequality (7.2). We prove this by considering the coefficients of each of the terms $n^{1+\gamma}$ and $n^{2\gamma}$.

Consider the $n^{1+\gamma}$ term first. It is easy to see that $a^{1+\gamma} + (1-a)^{1+\gamma} < 1$, because $1/2 \leq a \leq \alpha < 1$, and γ is positive. Furthermore, this expression attains its maximum when a is equal to α. Denote this maximum value by $\epsilon \equiv \alpha^{1+\gamma} + (1-\alpha)^{1+\gamma} < 1$. Equating the coefficients of $n^{1+\gamma}$ in the recurrence relation, if

$$C_1\epsilon + \alpha\beta(1+\Delta) \leq C_1,$$

then the first term in the claimed asymptotic bound on $E(n)$ would be true. Both this inequality and the condition on C_1 imposed by n_0 are satisfied if we choose

$$C_1 \geq \max\{\frac{\alpha\beta(1+\Delta)}{1-\epsilon}, (n_0+1)/2\}.$$

We simplify the coefficient of the $n^{2\gamma}$ term a bit before proceeding to analyze it. We have

$$\begin{aligned} & a^{2\gamma}\log an + (1-a)^{2\gamma}\log(1-a)n \\ \le\quad & a^{2\gamma}\log an + (1-a)^{2\gamma}\log an \;\le\; \left(\alpha^{2\gamma} + (1-\alpha)^{2\gamma}\right)\log\alpha\, n \;\equiv\; \theta\log\alpha\, n \\ \le\quad & \log\alpha\, n. \end{aligned}$$

In the transformations we have used the following facts: $1-a \le a$, since $a \ge 1/2$; the maximum of $a^{2\gamma} + (1-a)^{2\gamma}$, when $1/2 \le a \le \alpha$ and 2γ is greater than or equal to one, is attained for $a = \alpha$; this maximum value θ is less than one. Hence for the claim to hold, we require

$$C_2 \log\alpha\, n + \beta^2(1+\Delta) \le C_2\log n.$$

This last inequality is satisfied if we choose

$$C_2 \ge \frac{\beta^2(1+\Delta)}{\log\alpha^{-1}}.$$

□

A similar proof yields $\mathrm{Wbound}_{\min}(G) = \mathcal{O}(n^{2+\gamma})$, which is an upper bound on the work in an envelope-Cholesky factorization. Hence good separators imply small envelope size and work. Although we have used a "modified nested dissection" ordering to prove asymptotic upper bounds, we do not advocate the use of this ordering for envelope-reduction. Other envelope-reducing algorithms considered in this paper are preferable, since they are faster and yield smaller envelope parameters.

7.2. Asymptotic behavior of lower bounds. In this subsection we consider the implications of the spectral lower bounds that we have obtained. We denote the eigenvalue $\lambda_2(Q)$ by λ_2 for the sake of brevity in this subsection. We use the asymptotic behavior of the second eigenvalues together with the lower bounds we have obtained to predict the behavior of envelope parameters. For the envelope size, we make use of Theorem 3.2; for the envelope work, we employ Theorem 3.3.

The bounds on envelope parameters are tight for dense and random graphs (matrices). For instance, the full matrix (the complete graph) has $\lambda_2 = \Delta + 1 = n$, and hence $\mathrm{Esize}_{\min}(A) = \Theta(n^2)$. Similarly, the bound on the envelope work $\mathrm{Ework}_{\min}(A) = \Theta(n^3)$. The predicted lower bound is within a factor of three of the envelope size. These bounds are also asymptotically tight for random graphs where each possible edge is present in the graph with a given constant probability p, since the second Laplacian eigenvalue satisfies [23]

$$\lambda_2 = pn - \Theta([p(1-p)n\ \log n]^{1/2}).$$

More interesting are the implications of these bounds for degree-bounded finite element meshes in two and three dimensions. We will employ the following result proved recently by Spielman and Teng [38].

THEOREM 7.2. *The second Laplacian eigenvalue of an overlap graph embedded in d-dimensions is bounded by $\mathcal{O}(n^{-2/d})$.* □

problem	separator size	λ_2	Esize(A) LB	Esize(A) UB	Ework(A) LB	Ework(A) UB
d-dim.	$\mathcal{O}(n^{1-1/d})$	$\Theta(n^{-2/d})$	$\Omega(n^{2-2/d})$	$\mathcal{O}(n^{2-1/d})$	$\Omega(n^{3-4/d})$	$\mathcal{O}(n^{3-1/d})$

TABLE 7.1

Asymptotic upper and lower bounds on envelope size and work for an overlap graph in d dimensions.

Planar graphs are overlap graphs in 2 dimensions, and well-shaped meshes in 3 dimensions are also overlap graphs with $d = 3$.

Table 7.1 summarizes the asymptotic lower and upper bounds on the envelope parameters for a well-shaped mesh embedded in d dimensions. The most useful values are $d = 2$ and $d = 3$. As before, the lower bound on the envelope size is from Theorem 3.2, while the lower bound on the envelope work is from Theorem 3.3. The upper bound on the envelope size follows from Theorem 7.1, and the upper bound on envelope work follows from the upper bound on Wbound(A), discussed at the end of the proof of that theorem.

The lower bounds are obtained *for problems where the upper bounds on the second eigenvalue are asymptotically tight.* This is reasonable for many problems, for instance model problems in Partial Differential Equations. Note that the regular finite element mesh in a discretization of Laplace's equation in two dimensions (Neumann boundary conditions) has $\lambda_2 = \Theta(h^2) = \Theta(n^{-1})$, where h is the smallest diameter of an element (smallest mesh spacing for a finite difference mesh). The regular three-dimensional mesh in the discretized Laplace's equation with Neumann boundary conditions satisfies $\lambda_2 = \Theta(h^2) = \Theta(n^{-2/3})$.

For planar problems, the lower bound on the envelope size is $\Omega(n)$, while the upper bound is $\mathcal{O}(n^{1.5})$. For well-shaped three-dimensional meshes, these bounds are $\Omega(n^{4/3})$ and $\mathcal{O}(n^{5/3})$. The lower bounds on the envelope work are weaker since they are obtained from the corresponding bounds on the envelope size. Direct methods for solving sparse systems have storage requirements bounded by $\mathcal{O}(n \log n)$ and work bounded by $\mathcal{O}(n^{1.5})$ for a two-dimensional mesh; in well-shaped three dimensional meshes, these are $\mathcal{O}(n^{4/3})$ and $\mathcal{O}(n^2)$.

These results suggest that when a two-dimensional mesh possesses a small second Laplacian eigenvalue, envelope methods may be expected to work well. Similar conclusions should hold for three-dimensional problems when the number of mesh-points along the third dimension is small relative to the number in the other two dimensions, and for two-dimensional surfaces embedded in three-dimensional space.

8. Computational results. We present computational results to verify how well the spectral ordering reduces the 2-sum. We report results on two sets of problems.

The first set of problems, shown in Table 8.1, is obtained from John Richardson's (Thinking Machines Corporation) program for triangulating the sphere. The spectral lower bounds reported are from Theorem 5.2. Gap is the ratio with numerator equal to the difference between the 2-sum and the lower bound, and the denominator equal to the 2-sum. The results show that the spectral reordering algorithm computes values within a few percent of the optimal 2-sum, since the gap between the spectral 2-sum and the lower bound is within that range.

$\lvert V \rvert$	$\lvert E \rvert$	λ_2	Spectral LB	Spectral 2-sum	Gap(%)
18	48	2.00	969	978	0.9
66	192	6.25e-1	1.50e+4	1.54e+4	2.6
258	768	1.65e-1	2.36e+5	2.53e+5	6.9
1,026	3,072	4.17e-2	3.75e+6	4.05e+6	7.4
4,098	12,270	1.05e-2	6.00e+7	6.44e+7	7.3
16,386	49,152	2.60e-3	0.953e+9	1.03e+9	9.1

TABLE 8.1
2-sums from the spectral reordering algorithm and lower bounds for triangulations of the sphere.

Problem	$\lvert V \rvert$	$\lvert E \rvert$	λ_2	Spectral LB	Spectral 2-sum	Gap(%)
CAN1072	1,072	5,686	7.96e-2	8.17e+6	9.02e+6	9.4
NASA1824	1,824	18,692	2.71e-1	1.37e+8	1.74e+8	21
NASA2146	2,146	35,052	1.35e-1	1.11e+8	1.32e+8	16
NACA	4,224	12,416	3.57e-3	2.24e+7	2.70e+7	17
BARTH4	6,019	17,473	1.76-3	3.19e+7	5.41e+7	41
BARTH	6,691	19,748	2.62e-3	6.54e+7	6.69e+7	2.2
BARTH5	15,606	45,878	7.41e-4	2.35e+8	3.06e+8	23
BCSSTK30	28,924	1,007,284	1.96e-2	3.00e+10	5.73e+10	48
COPTER2	55,476	352,238	6.77e-3	9.63e+10	1.17e+11	18

TABLE 8.2
2-sums from the spectral reordering algorithm and lower bounds for some problems from the Boeing-Harwell and NASA collections.

Table 8.2 contains the second set of problems, taken from the Boeing-Harwell and NASA collections. Here the bounds are weaker than the bounds in Table 8.1. These problems have two features that distinguish them from the sphere problems. Many of them have less regular degree distributions—e.g., NASA1824 has maximum degree 41 and minimum degree 5. They also represent more complex geometries. Nevertheless, these results imply that the spectral 2-sum is within a factor of two of the optimal value for these problems. These results are somewhat surprising since we have shown that minimizing the 2-sum is NP-complete.

The gap between the computed 2-sums and the lower bounds could be further reduced in two ways. First, a local reordering algorithm applied to the ordering computed by the spectral algorithm might potentially decrease the 2-sum. Second, the lower bounds could be improved by incorporating diagonal perturbations to the Laplacian.

9. Conclusions. The lower bounds on the 2-sums show that the spectral reordering algorithm can yield nearly optimal values, in spite of the fact that minimizing the 2-sum is an NP-complete problem. To the best of our knowledge, these are the first results providing reasonable bounds on the quality of the orderings generated by a reordering algorithm for minimizing envelope-related parameters. Earlier work had not addressed the issue of the quality of the orderings generated by the algorithms. Unfortunately the tight bounds on the 2-sum do not lead to tight bounds on the envelope parameters. However, we have shown that problems with bounded separator sizes have bounded envelope parameters and have obtained asymptotic lower and upper bounds on these parameters for finite element meshes.

Our analysis further shows that the spectral orderings attempt to minimize the 2-sum rather than the envelope parameters. Hence a reordering algorithm could be used in a post-processing step to improve the envelope and wavefront parameters from a spectral ordering. A combinatorial reordering algorithm called the Sloan algorithm has been recently used to reduce envelope size and front-widths by Kumfert and Pothen [25]. Currently this algorithm computes the lowest values of the envelope parameters on a collection of finite element meshes.

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`http://cs.berkeley.edu/~spielman/spect.html`.

Appendix

A. Lower bounds on the minimum p-sum. We prove two lower bounds on the minimum p-sums. We make use of Lemma 3.1 in proving the first result. In the following $B_m(x)$ is the mth Bernoulli polynomial, and B_m is the mth Bernoulli number.

THEOREM A.1. *For $1 \leq p < \infty$, the minimum p-sum of a graph G on n vertices satisfies*

$$\sigma^p_{p,\min}(G) \geq \frac{1}{p+1}\left(B_{p+1}(s+1) - B_{p+1}\right),$$

where $s = (\lambda_2/4\Delta)n$.

Proof. Consider any ordering α of the vertices of G. Partition the vertices into two sets: A consisting of the lowest-numbered $n/2$ vertices, and B consisting of the highest-numbered $n/2$ vertices. By Lemma 3.1 the number of edges joining A and B, $|\delta(A,B)|$, is

$$|\delta(A,B)| \geq \frac{\lambda_2}{n}(n/2)^2.$$

Hence at least $s = |\delta(A,B)|/\Delta$ vertices in B are adjacent to vertices in A. Each vertex in this subset of B has the least row-width when it is adjacent to the highest-numbered vertex in A and to no other vertices in A. Hence these s vertices make a contribution of at least $1^p + \ldots + s^p$ to the p-sum, and this sum can be expressed in terms of the Bernoulli polynomials as stated. $\square$

From an expansion of the Bernoulli polynomial, we find that asymptotically

$$\sigma^p_{p,\min}(G) \geq \frac{1}{(p+1)(4\Delta)^{p+1}}{\lambda_2}^{p+1}n^{p+1} + \mathcal{O}(({\lambda_2}^p/\Delta^p)n^p).$$

We proceed to obtain another lower bound on the minimum p-sum.

The next result makes use of the following Lemma A.2 recently proved by Helmberg et al. [20]. Define the following symmetric function of the two positive integers m_1, m_2 (with $m_1 + m_2 < n$) and parameters λ_2, λ_n:

$$\text{(A.1)} \quad f(m_1,m_2) = \frac{\sqrt{m_1 m_2}}{2n}\left[\left(\sqrt{m_1 m_2} + \sqrt{(n-m_1)(n-m_2)}\right)\lambda_2 + \left(\sqrt{m_1 m_2} - \sqrt{(n-m_1)(n-m_2)}\right)\lambda_n\right].$$

LEMMA A.2. *Let S_1, S_2 be two disjoint subsets of the vertices of a graph G on n vertices, with $|S_i| = s_i$, for $i = 1, 2$. Then the number of edges joining S_1 and S_2, $|\delta(S_1,S_2)|$, satisfies*

$$|\delta(S_1,S_2)| \geq f(s_1,s_2). \quad \square$$

THEOREM A.3. *For $1 \leq p < \infty$, the minimum p-sum of a graph G satisfies*

$$\sigma^p_{p,\min}(G) \geq \frac{1}{2^{p+1}\Delta}\frac{{\lambda_2}^{p+1}}{(\lambda_n+\lambda_2)^{p+2}}(2\lambda_n+\lambda_2)(\lambda_n+2\lambda_2)n^{p+1}.$$

Proof. Consider any ordering α of the vertices of G, and consider a tripartition A, B, C: We choose A to consist of the lowest-numbered $a \equiv (n-b)/2$ vertices, C to consist of the highest-numbered $(n-b)/2$ vertices, and B to contain the remaining b vertices in the 'middle'. Here b, the size of B, is a parameter that will be determined later to obtain a large lower bound.

From Lemma A.2, $|\delta(A,C)|$, the number of edges joining A and C, is at least $f(a,a)$, where the symmetric function $f(.,.)$ is defined in (A.1). Hence there are at least $s_C = f(a,a)/\Delta$ vertices in C adjacent to vertices in A. Each of these vertices has row-width at least b.

Initially, consider the contribution to the envelope size Esize(G) made by these vertices to obtain a suitable value for b.

$$\begin{aligned} \text{(A.2)} \qquad \mathrm{Esize}(G) &\geq \frac{f(a,a)}{\Delta} b \\ &= \frac{(n-b)}{4n}\left[\left(\frac{n-b}{2}+\frac{n+b}{2}\right)\lambda_2 + \left(\frac{n-b}{2}-\frac{n+b}{2}\right)\lambda_n\right]\frac{b}{\Delta} \\ &= \frac{1}{4\Delta} b(n-b)\left(\lambda_2 - (b/n)\lambda_n\right). \end{aligned}$$

We choose b to maximize the lower bound on the envelope size. Differentiating the cubic polynomial in (A.2) with respect to b and simplifying, we obtain the quadratic equation

$$b^2 - \frac{2}{3}\frac{\lambda_2+\lambda_n}{\lambda_n} nb + \frac{1}{3}\frac{\lambda_2}{\lambda_n} n^2 = 0.$$

From the quadratic we find that the maximizer is, to first order, $b_m = (1/2)(\lambda_2/(\lambda_n+\lambda_2))n$.

Now we consider the contribution to the p-sum made by the s_C vertices in C adjacent to vertices in A. Each of these vertices contributes at least b^p to the p-sum, and thus a lower bound on the minimum p-sum is

$$\sigma^p_{p,\min}(G) \geq \frac{1}{4\Delta}(n-b)\left(\lambda_2 - (b/n)\lambda_n\right) b^p.$$

It is not easy to find a maximizer of the right-hand-side in the bound above on the p-sum since the polynomial in b is of degree $p+2$. Hence we choose b equal to the maximizer of the envelope size. We obtain the bound stated in theorem by substituting $b = b_m$ in the bound above. □

Juvan and Mohar [24] have proved upper bounds for the p-sums. The techniques in this Appendix can be used to compute bounds on Esize(A) and Wbound(A), but the results are weaker than those obtained in Section 3.