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ANALYSIS OF THE 2-SUM PROBLEM AND THE SPECTRAL ALGORITHM

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Abstract: *This paper presents the analysis of the 2-sum problem and the spectral algorithm. The spectral algorithm was proposed by Barnard, Pothen and Simon in [1]; its heuristic properties have been advocated by George and Pothen in [4] by formulation of the 2-sum problem as a Quadratic Assignment Problem. In contrast to that analysis another approach is proposed: permutations are considered as vectors of Euclidian space. This approach enables one to prove the bound results originally obtained in [4] in an easier way. The geometry of permutations is considered in order to explain what are 'good' and 'pathological' situations for the spectral algorithm. Upper bounds for approximate solutions generated by the spectral algorithm are proved. The results of numerical computations on (graphs of) large sparse matrices from real-world applications are presented to support the obtained results and illustrate considerations related to the 'pathological' cases.*

Keywords: *2-sum problem, Spectral Algorithm, Fiedler vector, Laplacian of a graph, graph layout problems, sparse matrices, spectral graph theory.*

1. INTRODUCTION

The 2-sum problem (to be defined in section 2) is one of the graph enumeration problems (also known as graph layout problems). Besides its purely theoretical interest, it was used as an approximation for large-scale graph labeling problems, that are important in numerical computations using large sparse matrices. Barnard, Pothen and Simon proposed spectral algorithm for envelope reduction of sparse matrices [1]. In fact, their algorithm yields an approximate solution of a 2-sum problem, which itself is used as an approximation for reducing envelope and envelope-related parameters of large sparse matrices. The spectral approach has also been used in the graph partitioning for finding the pseudoperipheral nodes of graphs, and other similar or related problems (e.g. [5,8]).

Fiedler studied the properties of the second Laplacian eigenvalue and eigenvector (also called Fiedler vector, i.e. eigenvector of Laplacian of a connected graph that corresponds to the second smallest eigenvalue). He observed that the differences between the components of this eigenvector are an approximate measure of the distance between the vertices [2,3]. Juvan and Mohar advocated the use of this eigenvector to compute bandwidth and p-sum (more general problem then 2-sum) reducing orderings [6]. [7] is a survey of the applications of Laplacian spectra to different combinatorial problems.

An approximate solution computed by spectral algorithm, generally, is only a heuristic approximation as the 2-sum problem was proved to be NP-complete [4]. Nevertheless, solutions generated by spectral algorithm are known to be quite good for minimizing the envelope of many real-world large sparse matrices [1].

In the paper [4], which is companion-paper for [1], George and Pothen provide analysis of spectral algorithm via Quadratic Assignment Problem (QAP). They formulate 2-sum problem as QAP, and analyze it utilizing permutation matrices. In this paper a different approach is presented (section 3) which instead considers permutations as Euclidian space vectors. Additionally, we present analysis of how effective or ineffective spectral algorithm can be for minimizing the 2-sum problem itself (not necessarily for envelope-reduction); as well as considerations leading to 'pathological' cases are provided. In section 4, computational results are presented to illustrate and test ideas from section 3 on Laplacians of graphs associated with real-world large sparse matrices.

The following notation is used throughout the paper: the underscore symbol _ indicates that the underlined letter is a column-vector (for example

$\underline{x}$); $\underline{u}$ is a column-vector all of whose components are 1.

If otherwise not mentioned, all vectors considered are non-zero column-vectors with dimension n; $n \geq 3$; some of the following considerations may not be correct for degenerate dimensions $n = 1$ and $n = 2$. The distance between vectors is as per Euclidian norm.

2. 2-SUM PROBLEM AND SPECTRAL ALGORITHM

In this section spectral algorithm is presented mainly following Barnard, Pothen and Simon's original work [1]; and as advocated by George and Pothen in [4].

We will consider connected and undirected graphs. Any graph of this type is associated with a symmetric matrix according to the following rule: there is an edge in the associated graph between vertices i and j if and only if the element a_{ij} of matrix A is nonzero. We will consider only matrices that have connected associated graphs.

Let us denote the column indices of the nonzero elements in the lower triangular part of the i-th row:

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

In these terms the 2-sum problem can be formulated as follows:

$$\sigma_2^2 = \sum_{i=1}^{n} \sum_{j \in row(i)} (i - j)^2 \tag{2.1}$$

i.e. the sum of squares of the differences between the vertices numbers which are in pairs that share a common edge in the corresponding associated graph. Hereinafter, the 2-sum problem will denote the problem of finding enumeration of graph vertices that minimizes (2.1). Obviously, the set of possible solutions to this problem is a set of permutations; let P denote the set of all permutations with length n.

The Laplacian matrix Q of an undirected graph G is the $n \times n$ matrix $(D - B)$ where D is the diagonal degree matrix, and B is the adjacency matrix of G. Laplacian matrix Q could be defined directly in terms of matrix A as:

$$q_{ij} = \begin{cases} -1, & i \neq j \;\; and \;\; a_{ij} \neq 0 \\ 0, & i \neq j \;\; and \;\; a_{ij} = 0 \\ -\sum_{\substack{j=1 \\ j \neq i}}^{n} q_{ij}, & i = j \end{cases} \tag{2.2}$$

The eigenvalues of Q are the Laplacian eigenvalues of G, and we list them as $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. An eigenvector corresponding to λ_k will be denoted by $\underline{x}_k$, and called a k-th eigenvector of Q. It is well-known that Q is a singular M-matrix, and hence its eigenvalues are nonnegative. Thus, $\lambda_1 = 0$, and the corresponding eigenvector is any nonzero constant vector. If G is connected, then Q is irreducible, and $\lambda_2 > 0$ (in the following we suppose that G is connected, otherwise 2-sum problem could be solved separately on each connected component).

Note the following properties of matrix Q that are used later, but not separately specified there:

1. $\underline{x}^T Q \underline{y} = \underline{y}^T Q \underline{x}$ (as Q is symmetrical);
2. $Q\underline{u} = \underline{u}^T Q = 0$ (by the definition of Q).

The idea is to consider the related 2-sum problem, and then show that a second Laplacian eigenvector $\underline{x}_2$ solves a continuous relaxation of the problem. Then it will be proved that the permutation vector, computed by spectral algorithm, is the closest vector among the permutation vectors to eigenvector $\underline{x}_2$. In [1] the following considerations have been proposed.

For odd n, let T denote the set of vectors whose components are permutations of $\{-(n-1)/2, \ldots, -1, 0, 1, \ldots, (n-1)/2\}$. For even n, let T denote vectors that are permutations of $\{-n/2, \ldots, -1, +1, \ldots, n/2\}$. Consider the 2-sum of a symmetric matrix A, defined with respect to vectors in T:

$$\sigma_2^2 = \frac{1}{2} \sum_{a_{ij} \neq 0} (t_i - t_j)^2 \to \min, \;\; t \in T \tag{2.3}$$

Note that any $\underline{t} \in T$ satisfies $\underline{t}^T u = 0$ and $l \equiv \underline{t}^T \underline{t} = (n/12)(n^2 - 1)$ for odd n, and $l \equiv \underline{t}^T \underline{t} = (n/12)(n+1)(n+2)$ for even n. Given a vector $\underline{x} \in R^n$, let us define permutation vector t *induced* by x by the rule $t_i \leq t_j$ if and only if $x_i \leq x_j$. Hence, to obtain a continuous relaxation of the discrete problem, consider the set of vectors $x \in R^n$ satisfying $x \neq 0, x^T u = 0$ and $x^T x = l$. This becomes the continuous optimization problem:

$$\frac{1}{2} \min_{x \in X} \sum_{a_{ij} \neq 0} (x_i - x_j)^2 =$$

$$= \min_{x \in X} \left(\sum_{i=1}^{n} d_i x_i^2 - 2 \sum_{\substack{j<i \\ a_{ij} \neq 0}} x_i x_j \right)$$

$$= \min_{x \in X} x^T Dx - x^T Bx = \min_{x \in X} x^T Qx$$
$$= \lambda_2 x_2^T x_2 = \lambda_2 l. \qquad (2.4)$$

Hence, a second Laplacian eigenvector $\underline{x}_2$ solves the continuous approximation of the 2-sum problem.

Spectral Algorithm (for 2-sum problem):

Step 1. Given a graph G, generate the Laplacian matrix Q.

Step 2. Compute a second eigenvector $\underline{x}_2$ of Q.

Step 3. Generate a permutation induced by $\underline{x}_2$.

Consider inducing more generally. Vectors $\underline{x}$ and $\underline{y}$ *are in an inducing relation*, (or equivalently: $\underline{x}$ induces $\underline{y}$, or $\underline{y}$ induces $\underline{x}$) if $y_i \le y_j$ if and only if $x_i \le x_j$; and at the same time, there are no additional restrictions on vectors introduced by this inducing relation. Obviously, inducing relation introduces reflexive, symmetric and transitive properties i.e. it is the equivalence relation on a set of vectors, none of which have identical components.

Lemma 2.1. Let there be vector $\underline{y}$ and a set Z that consists of $n!$ vectors, representing all possible permutations of any fixed set of components.

Then, vector $\underline{z} \in Z$, induced by vector $\underline{y}$, is closest to $\underline{y}$ among all vectors of set Z. If vector $\underline{y}$ induces several vectors from Z, then all of them will be at the same distance from $\underline{y}$.

Proof. By the definition of Euclidian norm:

$$\|\underline{y} - \underline{z}\| = \sqrt{\underline{y}^T \underline{y} + \underline{z}^T \underline{z} - 2\underline{y}^T \underline{z}} \qquad (2.5)$$

Since vectors from Z differ only in their component permutation, and vector $\underline{y}$ is fixed, scalar products $\underline{y}^T \underline{y}$ and $\underline{z}^T \underline{z}$ are positive constants, and $\underline{z}^T \underline{z}$ does not depend on the choice of $\underline{z}$. Therefore, in order to minimize the distance $\|\underline{y} - \underline{z}\|$ vector $\underline{z}$ has to maximize scalar product $\underline{y}^T \underline{z}$. Let us prove that this is true only if vector $\underline{z}$ is induced by vector $\underline{y}$. By contradiction: take a vector $\underline{\hat{z}} \in Z$, which is not in inducing relation with vector $\underline{y}$. Therefore, at least for the two components $\hat{z}_i$ and $\hat{z}_j$ of this vector, it is true that $\hat{z}_i < \hat{z}_j$ i.e. $\hat{z}_j = \hat{z}_i + a$, $a > 0$ and $y_i > y_j$. Now, scalar product $\underline{y}^T \underline{\hat{z}}$ increases if components $\hat{z}_i$ and $\hat{z}_j$ are swapped, while the other components remain in their places:

$$y_i \hat{z}_i + y_j \hat{z}_j = y_i(\hat{z}_j - a) + y_j(\hat{z}_i + a) =$$
$$= y_i \hat{z}_j + y_j \hat{z}_i + a(y_j - y_i) < y_i \hat{z}_j + y_j \hat{z}_i$$

since $a > 0$ and $(y_j - y_i) < 0$.

Thus, vector $\underline{\hat{z}}$ does not maximize the scalar product $\underline{y}^T \underline{z}$; and, hence, proof by contradiction is completed.

One should note that if vector $\underline{y}$ induces several vectors from Z, then all of them (by definition of inducing relation) have the same value of scalar product with $\underline{y}$ i.e. will be at the same distance from it.

The lemma proven is a slightly more general analogue of the corresponding theorem from [1].

The set of permutations P contains vectors that can be obtained from each other by all-possible component permutations. Therefore, according to the proven lemma, the permutation induced by vector $\underline{x}_2$ is the closest to it among all permutations.

The heuristic idea of choosing the permutation closest to the accurate solution naturally has to be such that, given the close position of the permutation chosen to the accurate solution, the increase of the cost function (quadratic form of matrix Q) remains small enough.

3. ANALYSIS

This section presents the analysis of the 2-sum problem. It is performed by the author of this paper in a quite different way than those in papers [2] and [1] for exploring and justifying spectral algorithm.

Let us consider permutations as vectors in n-dimension Euclidian space; we will denote the set of permutations as P. The following identities for any $p \in P$ are elementary:

$$\begin{aligned} &1 + 2 + \ldots + n = \underline{p}^T \underline{u} = \frac{n(n+1)}{2}, \\ &1^2 + 2^2 + \ldots n^2 = \underline{p}^T \underline{p} = \frac{n(n+1)(2n+1)}{6} \end{aligned} \qquad (3.1)$$

Let V be a set of vectors $\underline{v} \in \mathrm{R}^n$:

$$\begin{cases} \underline{v}^T \underline{u} = \dfrac{n(n+1)}{2} \\ \underline{v}^T \underline{v} = \dfrac{n(n+1)(2n+1)}{6} \end{cases} \qquad (3.2)$$

It is obvious that $P \subset V$.

For further analysis of the 2-sum problem in the relaxed form we will use a set X of admissible solutions. X is a set of non-zero vectors $\underline{x} \in \mathrm{R}^n$, satisfying the following conditions:

$$\begin{cases} \underline{x}^T \underline{x} = 1 \\ \underline{x}^T \underline{u} = 0 \end{cases} \quad (3.3)$$

Note that all our further analyses can be similarly performed by considering the first constraint in a generalized form: $\underline{x}^T \underline{x} = l$ ($l \in \mathrm{R}, l \neq 0$). We suppose $l = 1$ for the purpose of laconic formulation.

Consider a mapping of set V onto set X :

$$\underline{x} = \alpha(\underline{v} + \beta\underline{u}), \quad \alpha, \beta \in \mathrm{R}, \alpha \neq 0 \quad (3.4)$$

By considering conditions (3.2) and (3.3) we can define constants α and β:

$$\begin{aligned} \underline{x}^T \underline{u} &= \alpha(\underline{v} + \beta\underline{u})^T \underline{u} = \\ &= \alpha(\frac{n(n+1)}{2} + \beta n) = 0 \end{aligned}, \quad (3.5)$$

and since $\alpha \neq 0$, we get $\beta = -\dfrac{n+1}{2}$.

Similarly we obtain:

$$\begin{aligned} &\underline{x}^T \underline{x} = \alpha^2 (\underline{v} + \beta\underline{u})^T (\underline{v} + \beta\underline{u}) = 1 \\ &\Rightarrow \alpha = \sqrt{\frac{12}{n(n^2-1)}} \end{aligned} \quad (3.6)$$

Note that the mapping (3.4) is an affine transformation that compresses and shifts vectors in V.

Now, when expressing $\underline{v}$ from (3.4), we can show the mapping inverse to (3.4) is in the following form:

$$\underline{v} = \frac{1}{\alpha}(\underline{x} - \alpha\beta\underline{u}) = \alpha'(\underline{x} + \beta'\underline{u}), \quad (3.7)$$

$$\begin{aligned} \alpha' &= \frac{1}{\alpha} = \sqrt{\frac{n(n^2-1)}{12}}, \\ \beta' &= -\alpha\beta = \sqrt{\frac{3(n+1)}{n(n-1)}} \end{aligned} \quad (3.8)$$

Let us denote as $\tilde{X}$ a set of images of the transformation (3.4), the preimages of which are permutations from P. Since $P \subset V$, then $\tilde{X} \subset X$. Let the elements of set $\tilde{X}$ be called *representatives* of the corresponding permutations.

Thus, mappings (3.4) and (3.7) define the one-to-one dependence between sets V and X (and between their subsets P and $\tilde{X}$).

Lemma 3.1. $\quad \underline{\breve{x}}^T Q \underline{\breve{x}} > \underline{\hat{x}}^T Q \underline{\hat{x}}$

if and only if $\quad \underline{\breve{v}}^T Q \underline{\breve{v}} > \underline{\hat{v}}^T Q \underline{\hat{v}}$;

and also $\quad \underline{\breve{x}}^T Q \underline{\breve{x}} = \underline{\hat{x}}^T Q \underline{\hat{x}}$

if and only if $\quad \underline{\breve{v}}^T Q \underline{\breve{v}} = \underline{\hat{v}}^T Q \underline{\hat{v}}$,

where $\underline{\breve{x}} = \alpha(\underline{\breve{v}} + \beta\underline{u})$; $\underline{\hat{x}} = \alpha(\underline{\hat{v}} + \beta\underline{u})$; $\underline{\breve{x}}, \underline{\hat{x}} \in X$; $\underline{\breve{v}}, \underline{\hat{v}} \in V$.

Proof follows from (3.4), (3.7) and the identity:

$$(\alpha(\underline{y} + \beta\underline{u}))^T Q(\alpha(\underline{y} + \beta\underline{u})) = \alpha^2 \underline{y}^T Q \underline{y} .$$

In view of Lemma 3.1 we can analyze the discrete 2-sum problem not on set P, but on set $\tilde{X}$ and, correspondingly, examine its continuous variant on set X :

$$\begin{cases} \underline{x}^T Q \underline{x} \to \min \\ \underline{x} \in X \end{cases} \quad (3.9)$$

This problem is similar to (2.3) and, according to the well-known theorem of Courant-Fischer, the minimum is reached on vector $\underline{x}_2$ i.e. the second eigenvector of matrix Q; and maximum on vector $\underline{x}_n$:

$$\min_{\underline{x} \in X} \{\underline{x}^T Q \underline{x}\} = \lambda_2 ; \quad \max_{\underline{x} \in X} \{\underline{x}^T Q \underline{x}\} = \lambda_n \quad (3.10)$$

This can also be shown in another way: by using the Lagrange method for finding the conditional extremum of a multivariable function.

According to the above choice of permutation induced by vector $\underline{x}_2$, on Step 3 of spectral algorithm, the later can be presented as two transfers:

1) Transfer from vector $\underline{x}_2$ to vector $\underline{\tilde{x}}^*$ from $\tilde{X}$, which is induced by $\underline{x}_2$ (i.e. is the closest to it in $\tilde{X}$ according to Lemma 2.1). Thus, an approximate solution of 2-sum problem on set $\tilde{X}$ is obtained.

2) Transfer from vector $\underline{\tilde{x}}^*$ to the permutation it represents, according to (3.7), i.e. approximate solution of the 2-sum problem on set P is obtained.

The above sets and representations allow us to derive a simple proof of the following theorem, which was initially proved in [4] but using another approach.

Theorem 3.1. The following upper and lower bounds hold for the 2-sum problem:

$$\begin{aligned} &(1/12)\lambda_2 n(n-1)(n+1) \leq \sigma_2^2 \leq \\ &\leq (1/12)\lambda_n n(n-1)(n+1) \end{aligned} .$$

Proof. Let us prove the lower bound. Since $\tilde{X} \subset X$:

$$\min_{\underline{\tilde{x}} \in \tilde{X}} \{\underline{\tilde{x}}^T Q \underline{\tilde{x}}\} \geq \min_{\underline{x} \in X} \{\underline{x}^T Q \underline{x}\},$$

and taking into account (3.10)

$$\min_{\underline{\tilde{x}} \in \tilde{X}} \{\underline{\tilde{x}}^T Q \underline{\tilde{x}}\} \geq \lambda_2 .$$

In view of Lemma 3.1 and Corollary 1 it is true that:

$$\min_{\underline{p}\in P}\{\underline{p}^T Q \underline{p}\} = (\alpha')^2 \min_{\tilde{\underline{x}}\in\tilde{X}}\{\tilde{\underline{x}}^T Q \tilde{\underline{x}}\} \geq (\alpha')^2 \lambda_2 .$$

The substitution of value α' from (3.8) concludes the proof of the lower bound for σ_2^2. The proof of the upper-bound is analogous.

For clearer illustration of the following argumentation let us present a geometric interpretation of sets X and $\tilde{X}$. The equation $\underline{x}^T \underline{x} = 1$ from (3.3) defines an n-dimensional hypersphere with radius 1 at the point of origin; and the equation $\underline{x}^T \underline{u} = 0$ defines an n-dimensional hyperplane that intersects the point of origin and is orthogonal to vector $c\underline{u}, c \in \mathrm{R}$. Thus, set X is an $(n-1)$-dimensional hypersphere that is obtained from the intersection of the n-dimensional hypersphere with the n-dimensional hyperplane that intersects its center. Fig.1 is an illustration of the case $n = 3$. Hereinafter hypersphere will simply be called a sphere.

A set $\tilde{X}$ represents an $(n-1)$-dimensional polyhedron, the vertices of which are located on sphere X. It is easy to show that the permutations closest to each other, are those obtained from each other by simply permuting a pair of their components that differ by value 1; for example, $(1,2,3,4)$ and $(1,3,2,4)$. Similarly, the representatives of the permutations closest to each other are obtained from each other by permuting one pair of components that differ by value α.

When $n = 3$ the permutations' representatives are the vertices of the planar hexagon shown in Fig.2 (this hexagon is, in fact, inscribed in the shaded circle shown in Fig.1); near the hexagon's vertices the corresponding permutations are indicated.

When $n = 4$ all permutations are located on the $n - 1 = 3$ dimensional sphere, illustrated in Fig.3. The pairs of permutations closest to each other are connected, with the edges forming the polyhedron. Note that Fig.3 is not a schematic picture, but a 3-dimensional visualization made using Matlab.

To calculate the 3-dimensional coordinates, all 4!=24 permutations were first mapped into set $\tilde{X}$ according to (3.4). Then in plane $\underline{x}^T \underline{u} = 0$, the orthonormalized basis was chosen comprising 3 vectors; and in this basis, the permutations are represented in 3 dimensions (the fourth component of all permutations is 0).

Note that since the mapping (3.7) is an affine transform, the above description of the permutations' representatives characterizes the geometry of the permutations themselves.

Now, let us analyze possible increase of cost function value in problem (3.9) when transferring from vector $\underline{x}_2$ to its nearest vector $\tilde{\underline{x}}^* \in \tilde{X}$. It should be noted that the distance between vectors on sphere X is, in fact, determined by the scalar product of these vectors because

$$\|\underline{x} - \underline{y}\| = \sqrt{(\underline{x}-\underline{y})^T(\underline{x}-\underline{y})} = \sqrt{2(1-\underline{x}^T \underline{y})},$$

where $\underline{x}, \underline{y} \in X$. According to (3.3) $\underline{x} \in X \Leftrightarrow -\underline{x} \in X$, and considering the nearest vectors, it is assumed that the scalar product of any pair of vectors belongs to $[0,1]$ (when transferring from $\underline{x}$ to $-\underline{x}$, the value of the quadratic form of matrix Q does not change).

If $\tilde{\underline{x}}^* \neq \underline{x}_2$, then vector $\tilde{\underline{x}}^*$ can be considered as located on the arc of sphere X, which connects $\underline{x}_2$ and some orthogonal to it vector $\underline{z} \in X$, $\underline{z}^T \underline{x}_2 = 0$ (see Fig. 4) :

$$\tilde{\underline{x}}^* = \frac{a\underline{x}_2 + (1-a)\underline{z}}{\|a\underline{x}_2 + (1-a)\underline{z}\|}, \quad a \in [0,1] \qquad (3.11)$$

Let us call vector $\underline{z}$ a *spherical orthogonal continuation* of vector $\underline{x}_2$ through vector $\tilde{\underline{x}}^*$.

From (3.11) by the definition

$$(\underline{x}_2^T \tilde{\underline{x}}^*)\|a\underline{x}_2 + (1-a)\underline{z}\| = a$$

and so

$$(\underline{x}_2^T \tilde{\underline{x}}^*)^2((a\underline{x}_2 + (1-a)\underline{z})^T(a\underline{x}_2 + (1-a)\underline{z})) = a^2$$

.

Therefore we can obtain the following equations:

$$(\underline{x}_2^T \tilde{\underline{x}}^*)^2 = \frac{a^2}{(a^2 + (1-a)^2)};$$
$$1 - (\underline{x}_2^T \tilde{\underline{x}}^*)^2 = \frac{(1-a)^2}{(a^2 + (1-a)^2)} \qquad (3.12)$$

Now, the cost function value of the problem (3.9) on vector $\tilde{\underline{x}}^*$ can be represented as follows using (3.12):

$$\tilde{\underline{x}}^{*T} Q \tilde{\underline{x}}^* = $$
$$= \frac{a^2\lambda_2 + (1-a)^2 \underline{z}^T Q \underline{z}}{a^2 + (1-a)^2} = \qquad (3.13)$$
$$= (\underline{x}_2^T \tilde{\underline{x}}^*)^2 \lambda_2 + (1 - (\underline{x}_2^T \tilde{\underline{x}}^*)^2)\underline{z}^T Q \underline{z}$$

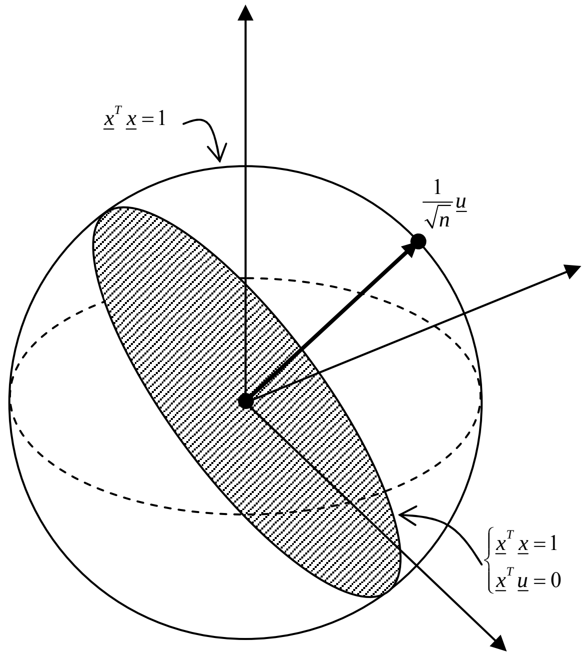

Fig. 1 – Geometry of the set X

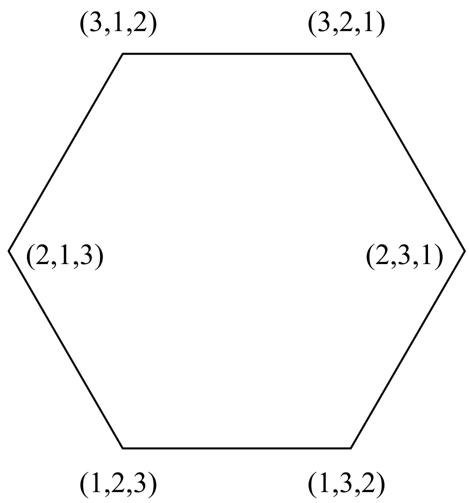

Fig. 2 – Geometry of permutation, n=3

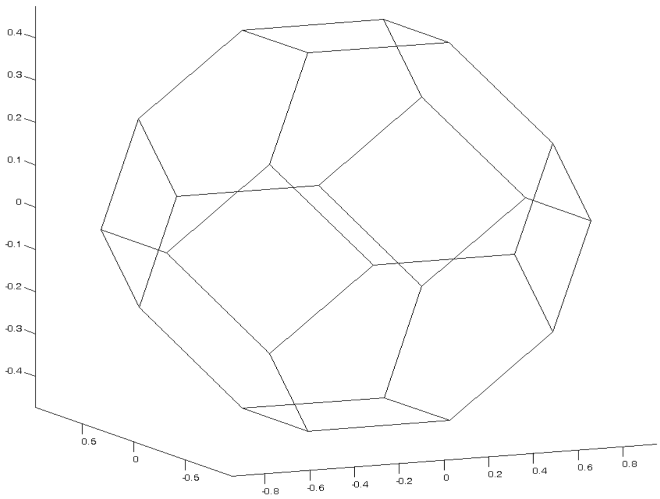

Fig. 3. Geometry of permutations, n=4

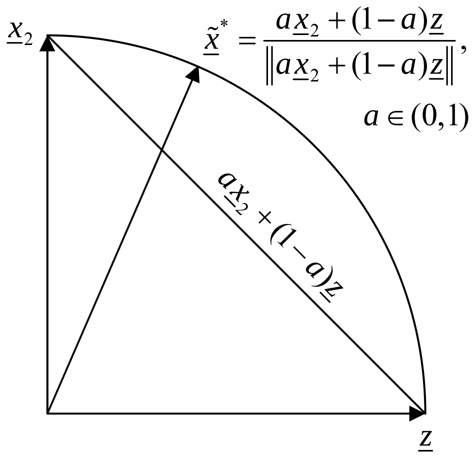

Fig. 4. Spherical combination

As easily seen from (3.13), it follows that the quadratic form of matrix Q strictly increases along the arc connecting $\underline{x}_2$ and $\underline{z}$; and with the fixed distance from $\underline{x}_2$ to $\tilde{\underline{x}}^*$, its value is defined by the value $\underline{z}^T Q \underline{z}$.

Thus, the increase of cost function value in problem (3.9), when transferring from $\underline{x}_2$ to $\tilde{\underline{x}}^*$, depends both on the distance from $\underline{x}_2$ to $\tilde{\underline{x}}^*$ (the bigger the distance, the bigger the function value), and on the direction in which such a transfer is performed (i.e. on cost function value on the spherical orthogonal continuation of vector $\underline{x}_2$ through vector $\tilde{\underline{x}}^*$).

Matrix Q is a normal matrix (because it is symmetric), so there is an orthogonal system formed by its eigenvectors. Setting $\underline{x}_1 = (1/\sqrt{n})\underline{u}$ an orthonormalized system of eigenvectors $\{\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_n\}$, $\underline{x}_i^T \underline{x}_j = 0 \quad (i \neq j)$ is obtained, that is a basis of the space R^n. In this basis, vector $\underline{\tilde{x}}^*$ is presented as follows:

$$\underline{\tilde{x}}^* = a_2 \underline{x}_2 + a_3 \underline{x}_3 + \ldots + a_n \underline{x}_n \tag{3.14}$$

because $\underline{\tilde{x}}^{*T} \underline{u} = 0$, and

$$\begin{aligned} &\underline{\tilde{x}}^{*T} \underline{\tilde{x}}^* = a_2^2 + a_3^2 + \ldots + a_n^2 = 1; \\ &(\underline{x}_i^T \underline{\tilde{x}}^*)^2 = a_i^2 \ \ (2 \le i \le n) \end{aligned} \tag{3.15}$$

From (3.14) and (3.15) it follows that

$$\begin{aligned} &\underline{\tilde{x}}^{*T} Q \underline{\tilde{x}}^* = \\ &= a_2^2 \lambda_2 + a_3^2 \lambda_3 + \ldots + a_n^2 \lambda_n \le \\ &\le a_2^2 \lambda_2 + (a_3^2 + \ldots + a_n^2) \lambda_n = \\ &= a_2^2 \lambda_2 + (1 - a_2^2) \lambda_n \end{aligned} \tag{3.16}$$

Note that we now come to the same result as in (3.13) if we suppose $\underline{z} = \arg\max_{\underline{x} \in X} \{\underline{x}^T Q \underline{x}\} = \underline{x}_n$.

Lemma 3.2. The following bound is true:

$$\begin{aligned} &(\underline{x}_2^T \underline{\tilde{x}}^*)^2 \lambda_2 + (1 - (\underline{x}_2^T \underline{\tilde{x}}^*)^2) \lambda_3 \le \underline{\tilde{x}}^{*T} Q \underline{\tilde{x}}^* \le \\ &\le (\underline{x}_2^T \underline{\tilde{x}}^*)^2 \lambda_2 + (1 - (\underline{x}_2^T \underline{\tilde{x}}^*)^2) \lambda_n \end{aligned}$$

where $\underline{\tilde{x}}^*$ is the nearest vector to $\underline{x}_2$ from $\tilde{X}$ (i.e. $\underline{x}_2$ induces $\underline{\tilde{x}}^*$).

Proof of the upper bound follows from (3.16) or from (3.13) using (3.10).

The lower bound follows from (3.13) if we suppose $\underline{z} = \arg\min_{\underline{x} \in X} \{\underline{x}^T Q \underline{x}\}$ with the additional restriction $\underline{x}^T \underline{x}_2 = 0$; in this case $\underline{z} = \underline{x}_3$ (as in (3.10) it follows from the Courant-Fischer theorem), and then $\underline{z}^T Q \underline{z} = \lambda_3$. □

Thus, the 'worst' transfer direction from $\underline{x}_2$ to $\underline{\tilde{x}}^*$ is an arc connecting $\underline{x}_2$ and $\underline{x}_n$, although it can be compensated by the nearness of $\underline{\tilde{x}}^*$ to $\underline{x}_2$.

Now, from the cost function decomposition in (3.16) it is clear that even after computing all eigenvectors/eigenvalues of the Laplacian Q, the problem of choosing a vector $\underline{\tilde{x}} \in \tilde{X}$, (even with guaranteed approximation) that minimizes $\underline{\tilde{x}}^T Q \underline{\tilde{x}}$ remains hard because the cost function depends on the squares of coefficients of vector $\underline{\tilde{x}}$ decomposition in the basis of Q eigenvectors.

Besides that, the computation of all eigenvectors/eigenvalues of large matrices is almost impossible in practice. Given this point of view, the heuristic idea of spectral algorithm consists in choosing $\underline{\tilde{x}}^*$, which maximizes $(\underline{x}_2^T \underline{\tilde{x}}^*)^2 = a_2^2$; owing to which one can expect a decrease in the coefficients corresponding to the bigger eigenvalues, and the value of the cost function will most likely be not much bigger than $\underline{x}_2^T Q \underline{x}_2 = \lambda_2$.

It is interesting to determine how far vectors $\underline{x} \in X$ and $\underline{\tilde{x}} \in \tilde{X}$, which are in inducing relation, can be distanced from each other. The following theorem answers this question.

Theorem 3.2. Let $\underline{\tilde{x}} \in \tilde{X}$ be induced by vector $\underline{x} \in X$ which has n_1 negative and n_2 positive components ($n_1 + n_2 = n$, and zero components are considered together with either negative or positive components). Then the following bound is true:

$$\underline{x}^T \underline{\tilde{x}} \ge \sqrt{\frac{3 n_1 n_2}{(n^2 - 1)}},$$

and equality is reached on the unique vector that has all positive components equal to each other and which stand on the same places as the positive components of vector $\underline{x}$; and where all negative components are equal to each other and stand on the same places as the negative components of vector $\underline{x}$.

The theorem has been proved by the author of this paper but the proof is too long and technical to present it here in full. The simplified scheme of the proof is the following:

1. Consider the theorem as the statement about the unique solution of the constrained minimization problem with the cost function $\underline{x}^T \underline{\tilde{x}}$.
2. Prove that the minimum exists.
3. Show that the minimum is unique.
4. Show that only the vector described in the second part of the theorem could be the minimum point.

From the geometrical point of view, the vectors which consist only of equal to each other positive and equal to each other negative components, pass through the 'centers' of the edges of the polyhedron of permutations representatives. So when $n = 4$ (see Fig. 3) the vectors $(-\sqrt{3/4}, \sqrt{1/12}, \sqrt{1/12}, \sqrt{1/12})$, $(-\sqrt{1/12}, -\sqrt{1/12}, -\sqrt{1/12}, \sqrt{3/4})$ and $(-\sqrt{1/4}, -\sqrt{1/4}, \sqrt{1/4}, \sqrt{1/4})$ pass through the centers of two hexagons and one quadrangle that share one vertex which is representative of unit permutation $\underline{p}_1 = (1, 2, 3, 4)$.

Evidently, the value of the bound we obtained in Theorem 3.2 reaches its maximum value when $n_1 = n_2 = n/2$ (approximately for odd n), and its minimum on the points $\{n_1 = 1, n_2 = n - 1\}$ and

$\{n_1 = n-1, n_2 = 1\}$. That is why with unknown n_1 and n_2 the following is true

Corollary 1 from Theorem 3.2. Let $\underline{\tilde{x}} \in \tilde{X}$ be induced by vector $\underline{x} \in X$, then

$$\underline{x}^T \underline{\tilde{x}} \geq \sqrt{\frac{3}{n+1}}.$$

Asymptotical behavior of the bound when $n \to \infty$ essentially depends on the ratio of n_1 and n_2:

If $n_1 = n_2 = \dfrac{n}{2}$,

then $\lim\limits_{n\to\infty} \sqrt{\dfrac{3n_1n_2}{(n^2-1)}} = \lim\limits_{n\to\infty} \sqrt{\dfrac{3n^2}{4(n^2-1)}} = \sqrt{\dfrac{3}{4}}$,

if $n_1 = 1, n_2 = n-1$ or $n_1 = n-1, n_2 = 1$ then

$$\lim_{n\to\infty} \sqrt{\frac{3n_1n_2}{(n^2-1)}} = \lim_{n\to\infty} \sqrt{\frac{(n-1)}{(n^2-1)}} = 0$$

i.e. in the 'worst case' (for example, if $n_1 = 1, n_2 = n-1$) vectors $\underline{x}^T$ and $\underline{\tilde{x}}$ are 'asymptotically orthogonal'.

Applying the Theorem 3.2 to $\underline{x}_2$ and $\underline{\tilde{x}}^*$ we obtain: $\underline{x}_2^T \underline{\tilde{x}}^* \geq \sqrt{\dfrac{3n_1n_2}{(n^2-1)}}$, where n_1 and n_2 correspondingly denote the number of positive and negative components in vector $\underline{x}_2$. Substituting this bound in the inequality of Lemma 3.2 we obtain:

$$\underline{\tilde{x}}^{*T} Q \underline{\tilde{x}}^* \leq \frac{3n_1n_2}{(n^2-1)}\lambda_2 + \left(1 - \frac{3n_1n_2}{(n^2-1)}\right)\lambda_n =$$

$$= \frac{1}{n^2-1}\left(3n_1n_2\lambda_2 + (n^2 - 3n_1n_2 - 1)\lambda_n\right) \quad (3.21)$$

Equality can be reached if in vector $\underline{x}_2$ all the negative components equal c and all the positive components equal k. Then all permutations where numbers $1, 2, \ldots, n_1$ stand on the same places as in c in $\underline{x}_2$, and numbers $n_1+1, \ldots, n$ stand on the same places as k in $\underline{x}_2$ are closest to $\underline{x}_2$ in P (in all there are $n_1!n_2!$ such permutations), and their representatives are closest to $\underline{x}_2$ in $\tilde{X}$. In this case spectral algorithm can choose any of these permutations and in the 'worst case' the chosen permutation will be located on the arc connecting $\underline{x}_2$ and $\underline{x}_n$.

The asymptotical behavior of the bound (3.21) also depends substantially on the relation between n_1 and n_2:

If $n_1 = n_2 = \dfrac{n}{2}$,

then $\lim\limits_{n\to\infty} \underline{\tilde{x}}^{*T} Q \underline{\tilde{x}}^* = \dfrac{3}{4}\lambda_2 + \dfrac{1}{4}\lambda_n$,

if $n_1 = 1, n_2 = n-1$ or $n_1 = n-1, n_2 = 1$,

then $\lim\limits_{n\to\infty} \underline{\tilde{x}}^{*T} Q \underline{\tilde{x}}^* = \lambda_n$.

Nevertheless, the above bounds are usually not reached on the graphs of big sparse matrices from real-world applications (as described in Section 4) because the above described 'pathological' situations are not realized. To the contrary, the value of the quadratic form $\underline{\tilde{x}}^{*T} Q \underline{\tilde{x}}^*$ usually is not much bigger than λ_2 while λ_n is several orders bigger than λ_2.

Nevertheless, strictly speaking, with a fixed n we have only a finite number of usual Laplacians, but there are infinitely many weighted ones, whose components can differ greatly. The above analysis can be applied to any Laplacian, including a weighted Laplacian. The obtained bounds still hold without additional restrictions being imposed on a graph, e.g. the degrees of its vertices need not be bounded.

4. COMPUTATIONAL RESULTS

This section lists the results obtained for examining and illustrating the performance of spectral algorithm on Laplacians of real-world large sparse matrices. The matrices used were taken from the Harwell-Boeing and NASA collections that are in Tim Davis' University of Florida Sparse Matrix Collection [9]. These matrices are often used for testing and comparing reordering algorithms for sparse matrices. All computations have been performed in Matlab 7 (Release 14, Service Pack 2); vectors $\underline{x}_2$ and $\underline{x}_n$ were computed using `eigs` function (as defined in Section 2, $\underline{x}_2$ and $\underline{x}_n$ are eigenvectors of the graph's Laplacian corresponding to the 2nd and the largest eigenvalues).

Table 1 presents the following data:

n is a matrix (graph) dimension;

$|E|$ is the number of edges of a graph ($2|E|+n$ is the number of the non-zero matrix elements);

Deg. min / max are minimum and maximum degrees of graph vertices;

pos./neg. values in $\underline{x}_2$ are numbers of positive and negative components in $\underline{x}_2$;

$F(\underline{x}_2)$, $F(\underline{\tilde{x}}^*)$, $F(z)$, $F(\underline{x}_n)$ are values of the Laplacian quadratic forms on the corresponding vectors; vector $\underline{z}$ is the spherical orthogonal continuation of vector $\underline{x}_2$ through vector $\underline{\tilde{x}}^*$ (these vectors were defined and discussed in Section 3);

$\underline{x}_2^T \underline{\tilde{x}}^*$ is the scalar product of vectors $\underline{x}_2$ and $\underline{\tilde{x}}^*$ that shows the nearness of $\underline{\tilde{x}}^*$ to $\underline{x}_2$.

Table 1. Experimentation with the real-world large sparse matrices (graphs)

Matrix	*n*	$\lvert E \rvert$	*Deg. min / max*	*pos./neg. values in* $\underline{x}_2$	$F(\underline{x}_2)$	$F(\underline{\tilde{x}}^*)$	$F(\underline{z})$	$F(\underline{x}_n)$	$\underline{x}_2^T \underline{\tilde{x}}^*$
CAN1054	1,054	5,571	5 / 34	558 / 496	5.93e-2	6.65e-2	8.56e-1	3.57e+1	0.995
CAN1072	1,072	5,686	5 / 34	480 / 592	7.96e-2	8.78e-2	6.11e-1	3.57e+1	0.992
BCSSTK15	1,505	5,406	3 / 34	90 / 1,415	4.24e-2	1.13e+0	1.35e+0	3.54e+1	0.418
NASA1824	1,824	18,692	5 / 41	913 / 911	2.71e-1	3.58e-1	5.21e+0	4.42e+1	0.991
NASA2146	2,146	35,052	13 / 35	1,066 / 1,080	1.35e-1	1.61e-1	1.88e+0	4.77e+1	0.992
NASA2910	2,910	85,693	15/ 174	1,634 / 1,276	1.10e+0	1.74e+0	1.62e+1	1.76e+2	0.978
NASA4704	4,704	50,026	5 / 41	2,438 / 2,266	8.26e-2	9.33e-2	2.36e+0	4.43e+1	0.998
BARTH4	6,019	17,473	3 / 12	3,453 / 2,566	1.77e-3	2.91e-3	2.13e-2	1.34e+1	0.970
BARTH	6,691	19,748	3 / 12	3,354 / 3,337	2.60e-3	2.68e-3	1.47e-1	1.34e+1	1.000
SHUTTLE_EDDY	10,429	46,585	3 / 26	5,389 / 5,040	6.23e-4	2.28e-3	4.86e-2	2.74e+1	0.983
BARTH5	15,606	45,878	3 / 10	6,816 / 8,790	7.70e-4	9.67e-4	5.55e-3	1.17e+1	0.979
BCSSTK30	28,924	1,007,284	3 / 218	15,428 / 13,496	1.95e-2	2.84e-2	5.68e-1	2.22e+2	0.992
BCSSTK32	44,609	985,046	1 / 215	7,079 / 37,530	6.00e-3	2.86e-2	5.15e-2	2.17e+2	0.71

As we can see from Table 1, in most cases the closest representative to $\underline{x}_2$ is very closely located (product $\underline{x}_2^T \underline{\tilde{x}}^*$ is close to 1); and the value of $F(\underline{\tilde{x}}^*)$ is not much bigger than $F(\underline{x}_2)$, at least $F(\underline{\tilde{x}}^*)$ is of the same order as $F(\underline{x}_2)$. At the end of an arc (on vector $\underline{z}$) the value $F(\underline{z})$ is at least one order bigger than the value $F(\underline{\tilde{x}}^*)$ i.e. for $F(\underline{\tilde{x}}^*)$ to be close to $F(\underline{x}_2)$ the nearness of $\underline{\tilde{x}}^*$ to $\underline{x}_2$ is important. At the same time, the value $F(\underline{x}_n)$ is in most cases at least one order bigger than $F(\underline{z})$, which indicates the relatively 'good' direction of shifting along the arc (compare in the 'worst' case $F(\underline{z}) = F(\underline{x}_n)$ i.e. the arc connects $\underline{x}_2$ and $\underline{x}_n$). The example of a very 'good' direction is BARTH5 ($F(\underline{z})$=5.55e-3; $F(\underline{x}_n)$=1.17e+1). It is interesting to note that matrices, where the above situation pertains, have a different size, structure and degree of sparseness. Some of them also have a very dispersed degrees of vertices in the associated graph (for example, in NASA2910 the minimum degree is 15, and maximum 174; with the relatively small dimension $n = 2,910$). Additionally, the close (in some cases almost equal) number of positive and negative components in vector $\underline{x}_2$ is common for these matrices.

A different situation pertains in BCSSTK32, and especially in BCSSTK15. In these $\underline{\tilde{x}}^*$ is located fairly far from $\underline{x}_2$. Because of this the value $F(\underline{\tilde{x}}^*)$ is much bigger than $F(\underline{x}_2)$ and has the same order as $F(\underline{z})$. These two matrices are characterized by a large number of components of one sign and a small number of another sign in $\underline{x}_2$; for BCSSTK15 the ratio is 90 : 1,415.

From the geometrical point of view when the numbers of positive and negative components in $\underline{x}_2$ are close, it is located on the sphere X 'above' 'small' edge of the polyhedron of permutations (see Fig. 3); and that's why we can expect the closest representative of permutation $\underline{\tilde{x}}^*$ to be located very closely ($\underline{x}_2^T \underline{\tilde{x}}^*$ is close to 1). Otherwise, $\underline{x}_2$ is located 'above' 'big' edge and, correspondent vector $\underline{\tilde{x}}^*$ can be located fairly far away ($\underline{x}_2^T \underline{\tilde{x}}^*$ are substantially smaller than 1). In the worst case, $\underline{x}_2$ could be located 'above' the center of the 'biggest' possible edge, and the bound from Corollary 1 of

Theorem 3.2 could be reached.

5. CONCLUSIONS

Spectral algorithm provides a good balance between the computational cost and the accuracy of the approximate solution obtained for NP-complete 2-sum problem. The analysis conducted shows that there are ‘pathological’ cases for spectral algorithm, and that these are due to the geometrical properties of permutations considered as vectors in Euclidian space. These conclusions are illustrated by the computational results obtained using Laplacians of graphs of big sparse matrices. It should be noted that spectral algorithm can even be used as an effective approximation algorithm for small dimensions graphs; for small graphs it is possible to compute all eigenvalues and eigenvectors, but this additional information would not fundamentally simplify the solution of a 2-sum problem in all cases.

The proposed ‘geometrical’ approach enables the simple proof of the upper and lower bounds of the 2-sum problem. Potentially it could turn out to be helpful for analysis or design of algorithms for other similar problems like p-sum, graph partitioning, etc.

To the author’s knowledge, it is the first time strict (non-trivial) upper bounds are derived for the cost function of a 2-sum problem on an approximate solution provided by spectral algorithm. As the computational experiment shows, these bounds are usually not reached on the graphs of real-world large sparse matrices because the ‘pathological’ cases are not realized or are realized only partially.

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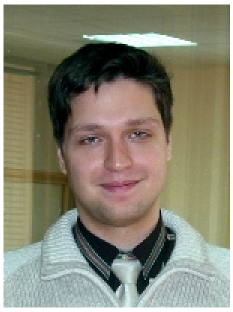

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