Characterizing Graph Drawing with Eigenvectors‡

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Two definitions of the problem of graph drawing are considered, and an analytical solution is provided for each of them. The solutions obtained make use of the eigenvectors of the Laplacian matrix of a related structure. The procedures give good results for symmetrical graphs, and they have already been used for drawing fullerene molecules in the literature. The analysis characterizes precisely what problems the two procedures are solving. It also illuminates why they can perform unsatisfactorily on asymmetrical graphs.

1. INTRODUCTION

We consider the problem of embedding a graph on n vertices in Euclidean space R^k, for $k < n$. Typically k would be 3 or 2. By posing the problem as minimizing the squared norm of the appropriately weighted distance between adjacent points subject to natural normalizing conditions, we arrive at a formulation of the problem for which the optimal solution can be simply computed in terms of the eigenvectors of the Laplacian matrix of the (weighted) graph. For the case where the weights are chosen to be unity, the solution is independent of the uniform penalty given to nonadjacent vertices. In this case and for regular graphs the technique has been applied by Pisanski,[9] who demonstrated that the generated drawings are particularly pleasing in the case of fullerene graphs arising in chemistry. The idea of using eigenvectors for drawing graphs was used first in chemical setting for molecular orbitals; see ref 8. A similar technique has been developed by Bolla[2] for generating Euclidean representations of hypergraphs. For distance-regular graphs with a second eigenvalue of multiplicity at least k, the embedding has interesting properties; see Godsil.[4]

This paper demonstrates that a problem that has been traditionally solved by gradient descent techniques used to minimize a measure of poverty of the generated embedding affords an analytical solution which can be implemented in an efficient deterministic algorithm.[9] At the same time it reveals significant insights into the relations between embeddings of graphs and the structure of the eigenspaces of their Laplacian matrices.

The Laplacian matrix has been used in graph embedding before in Tutte's straight-line embedding of planar graphs.[10,11] The approach presented here is related but corresponds to solving the equation without boundary conditions. The characterization in terms of minimizing the sum of distances between vertices is also appropriate in Tutte's case but subject to the chosen cycle being fixed at the boundary; see also Becker and Hotz.[1]

Use of eigenvectors to generate embeddings is not new. As early as 1980 Kruskal and Seery[6] devised a sophisticated method for drawing network diagrams using a statistical technique called multidimensional scaling (MDS)[5,7] to arrive at a matrix whose eigenvectors could be viewed as embedding vectors. The approach is closely related to that presented here, but is not characterized in terms of a tightly defined optimization problem. In section 4 we discuss in detail the relationship between their method and one of our techniques. It transpires that in certain special cases the solutions obtained by the two methods are up to scaling factors identical. The main advantage of our approach is the theoretical explanation in terms of the two optimization problems which elucidates the strengths and weaknesses of the two methods.

2. NOTATION AND KNOWN RESULTS

Let $A(G) = (A_{uv})$ be the adjacency matrix of a simple (positively weighted) n-vertex graph G with no loops. Note that u, v are understood to be adjacent if and only if $A_{uv} > 0$. For nonadjacent vertices $A_{uv} = 0$. Let D be the $n \times n$ diagonal matrix with nonzero entries

$$D_{vv} = \sum_{u:(u,v)\in E(G)} A_{uv}$$

the weighted degree of vertex v. The Laplacian matrix is defined to be $Q(G) = Q(A) = D - A$, where $A = A(G)$.

We summarize a few known results involving the Laplacian matrix. We will number the eigenvalues of $Q(G)$ given in ascending order: $0 = \lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$, with corresponding eigenvectors $\boldsymbol{j} = \boldsymbol{e}^1, \boldsymbol{e}^2, \ldots, \boldsymbol{e}^n$, where $\boldsymbol{j}$ is the all-1 vector, while $0 < \lambda_2$ if the graph is connected. In

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addition, for any n-dimensional real vector $\boldsymbol{x}$ it can be verified that

$$\boldsymbol{x}^{\mathrm{T}}Q(G)\boldsymbol{x} = \sum_{(u,v)\in E(G)} A_{uv}(\boldsymbol{x}_u - \boldsymbol{x}_v)^2 \qquad (1)$$

3. GRAPH DRAWING PROBLEM AND INITIAL RESULT

We pose the problem of embedding a graph G as finding a mapping

$$\tau : V(G) \rightarrow \mathrm{R}^k$$

We will place constraints on this mapping in order to ensure that the representation is natural and hopefully pleasing. We will denote by $\boldsymbol{\tau}_i$ the n-dimensional vector formed by taking the ith coordinate $\tau(u)_i$ of $\tau(u)$ for all $u \in V(G)$. Thus $\boldsymbol{\tau}_i$ is an n-dimensional vector indexed by the vertices of the graph G. Our first requirement is that the center of gravity of the representation be at the origin. This implies that the vectors $\boldsymbol{\tau}_i$ have average entry 0, or $\boldsymbol{\tau}_i \perp \boldsymbol{j}$, for $i = 1, ..., k$. The next constraint is that the scaling in all dimensions be similar. This is ensured by requiring that

$$||\tau_i||^2 = \sum_{u=1}^{n} \tau(u)_i^2 = 1.$$

Note that throughout this paper the norm notation $||\cdot||$ will as here refer to the 2-norm. Finally, we would like the embedding to retain maximum information about the graph. An example of how information can be lost is given when $\boldsymbol{\tau}_i = \boldsymbol{\tau}_j$ for some $i \neq j$, i.e., $\boldsymbol{\tau}_i$ and $\boldsymbol{\tau}_j$ are maximally correlated. In this case we have effectively reduced the dimension of the representation by one. Hence maximal information will be represented if the vectors have zero correlation, i.e., $\boldsymbol{\tau}_i \perp \boldsymbol{\tau}_j$, for $i \neq j$. We require adjacent vertices to be close together weighted according to A_{uv} (e.g., for different chemical bond types the value might vary), and we require nonadjacent vertices to be far apart. Our definition of the graph drawing problem may therefore be stated as follows.

Problem 3.1. *Graph drawing of an n-vertex graph G given by (weighted) adjacency matrix A in* R^k, $k < n$. Find a mapping $\tau : V(G) \rightarrow \mathrm{R}^k$, which minimizes the following energy function

$$E(\tau) = \sum_{(u,v)\in E(G)} A_{uv}||\tau(u) - \tau(v)||^2 - \beta \sum_{(u,v)\notin E(G)} ||\tau(u) - \tau(v)||^2$$

subject to the constraints

$$||\tau_i|| = 1, \boldsymbol{\tau}_i \perp \boldsymbol{j}, \quad \text{for } i = 1, ..., k$$

$$\boldsymbol{\tau}_i \perp \boldsymbol{\tau}_j, \quad \text{for } 1 \leq i < j \leq k$$

where β is a positive constant controlling the strength of the force driving nonadjacent vertices apart. ■

Before proceeding, some further discussion of our problem definition is warranted. First, there seems to be some arbitrariness in the fact that we can specify different "attractions" between vertices but nonadjacent vertices are all "repelled" with equal force. We will show that the more general problem created by allowing negative weights can also be solved using the techniques derived for problem 3.1.

Another aspect of the definition that is a little unsatisfactory is the requirement that the scaling be similar in all directions. Indeed we will see that the method does not work well for highly asymmetrical graphs. In order to avoid this artificial symmetrization we propose the following second definition of the graph drawing problem albeit with a similar flavor to problem 3.1.

Problem 3.2. *Graph drawing of an n-vertex graph G given by (weighted) adjacency matrix A in* R^k, $k < n$.

Find a mapping $\tau : V(G) \rightarrow \mathrm{R}^k$, such that the function

$$E(\boldsymbol{\tau}_i) = \sum_{(u,v)\in E(G)} A_{uv}|\tau(u)_i - \tau(v)_i|^2 - \beta \sum_{(u,v)\notin E(G)} |\tau(u)_i - \tau(v)_i|^2 = 1$$

for $i = 1, ..., k$, while maximizing the sum of the norms

$$\sum_{i=1}^{k} ||\boldsymbol{\tau}_i||^2 = \sum_{u\in V(G)} ||\tau(u)||^2$$

subject to the constraints

$$\boldsymbol{\tau}_i \perp \boldsymbol{j}, \quad \text{for } i = 1, ..., k$$

$$\boldsymbol{\tau}_i \perp \boldsymbol{\tau}_j, \quad \text{for } 1 \leq i < j \leq k$$

where β is a positive constant controlling the strength of the force driving nonadjacent vertices apart. ■

Note that this model allows the $\boldsymbol{\tau}_i$ to have different norms, but specifies that a unit length of "wire" is available in each dimension to create the model. Clearly changing the amount of wire simply has a scaling effect on the solution, so that the problem is well-posed if the number 1 is replaced by any constant. Note also that the requirement also implies that the amount of "wire" used is the same for all directions since the norms are sums of squares over the coordinates. This observation lends the definition a naturalness that matches the definition of problem 3.1.

We are now in a position to state our main result.

Theorem 3.1. *Let G be a connected n-vertex weighted graph with adjacency matrix A. The graph drawing problem given in problem 3.1 is solved by taking the weighted graph with adjacency matrix B with entries*

$$B_{uv} = \begin{cases} (A_{uv} + \beta) & \text{if } (u, v) \in E(G) \\ 0 & \text{otherwise} \end{cases}$$

and computing the eigenvectors $\boldsymbol{e}^1, \boldsymbol{e}^2, ..., \boldsymbol{e}^n$ *with corresponding eigenvalues* $0 = \lambda_1 < \lambda_2 \leq ... \leq \lambda_n$ *of the Laplacian matrix Q(B). An optimal embedding* τ *is given by* $\boldsymbol{\tau}_i = \boldsymbol{e}^{i+1}$, $i = 1, ..., k$ *and the minimal value of* $E(\tau)$ *is*

$$\sum_{l=2}^{k+1} \lambda_l - \beta nk$$

If $\lambda_{k+1} < \lambda_{k+2}$, *then the optimal embedding is unique up to orthogonal transformations in* R^k.

Corollary 3.1. *In the case where the graph is not weighted (i.e.,* $A_{uv} \in \{0,1\}$*), the optimal embedding does not depend on the parameter* β.

Proof: If the graph is not weighted and has adjacency matrix A, then $B = (1 + \beta)A$. Hence the Laplacian matrices $Q(A)$ and $Q(B)$ also satisfy $Q(B) = (1 + \beta)Q(A)$. This implies that they have the same eigenvectors with the corresponding eigenvalues of $Q(B)$ multiplied by a factor of $1 + \beta$. Hence by the theorem the optimal embedding does not depend on the parameter β. ■

Proof of Theorem 3.1. First note that we can rewrite the energy function $E(\tau)$ as follows.

$$E(\tau) = \sum_{(u,v)\in E(G)} (A_{uv} + \beta)\|\tau(u) - \tau(v)\|^2 - \beta \sum_{(u,v)\in E(K_n)} \|\tau(u) - \tau(v)\|^2 \quad (2)$$

where K_n is the complete graph on the vertices of G with edges weighted 1. If we consider the complete graph in eq 1, the following equality is obtained for an n-dimensional real vector $\boldsymbol{x}$.

$$\boldsymbol{x}^{\mathrm{T}}Q(K_n)\boldsymbol{x} = \boldsymbol{x}^{\mathrm{T}}(nI - J)\boldsymbol{x} = \sum_{u,v\in V(K_n)} (\boldsymbol{x}_u - \boldsymbol{x}_v)^2 \quad (3)$$

where I is the $n \times n$ identity matrix and J is the $n \times n$ all-1 matrix, i.e., $J_{ij} = 1$, for all i, j. In general we have the following relation for an embedding τ and graph G with adjacency matrix A and its Laplacian matrix $Q(A)$.

$$\begin{aligned}\sum_{(u,v)\in E(G)} A_{uv}\|\tau(u) - \tau(v)\|^2 &= \sum_{(u,v)\in E(G)} A_{uv}\sum_{i=1}^{k} (\tau(u)_i - \tau(v)_i)^2 \\ &= \sum_{i=1}^{k} \sum_{(u,v)\in E(G)} A_{uv}(\tau(u)_i - \tau(v)_i)^2 \\ &= \sum_{i=1}^{k} \boldsymbol{\tau}_i^{\mathrm{T}}Q(A)\boldsymbol{\tau}_i \quad (4)\end{aligned}$$

by eq 1. Combining the results of eqs 2−4, we obtain the following expression for the energy function $E(\tau)$.

$$E(\tau) = \sum_{i=1}^{k} \boldsymbol{\tau}_i[Q(B) - \beta(nI - J)]\boldsymbol{\tau}_i \quad (5)$$

Let $\boldsymbol{j} = \boldsymbol{e}^1, ..., \boldsymbol{e}^n$ be the eigenvectors of $Q(B)$ with corresponding eigenvalues $0 = \lambda_1 < \lambda_2 \leq ... \leq \lambda_n$. Without loss of generality we may take $\|\boldsymbol{e}^i\| = 1$ for $i > 1$, since eigenvectors are only determined up to their direction. Note that eigenvectors of a symmetric matrix are orthogonal and so $\boldsymbol{e}^i \perp \boldsymbol{e}^j$ for $i \neq j$. We have

$$[Q(B) - \beta(nI - J)]\boldsymbol{e}^1 = \boldsymbol{0}$$

while for $i > 1$, $\boldsymbol{e}^i \perp \boldsymbol{j}$ and so

$$[Q(B) - \beta(nI - J)]\boldsymbol{e}^i = (\lambda_i - \beta n)\boldsymbol{e}^i$$

Hence the eigenvectors of $Q(B)$ are also eigenvectors of $Q(B) - \beta(nI - J)$. Expressing $\boldsymbol{\tau}_i$ in the eigenbasis, we have

$$\boldsymbol{\tau}_i = \sum_{l=2}^{n} \mu_i^l \boldsymbol{e}^l$$

where $\mu_i^1 = 0$ since $\boldsymbol{\tau}_i \perp \boldsymbol{j}$ ($\boldsymbol{j} = \boldsymbol{e}^1$). Hence we can write the energy of τ as

$$\begin{aligned}E(\tau) &= \sum_{i=1}^{k}\sum_{l=2}^{n} (\mu_i^l)^2\lambda_l - \beta nk \\ &= \sum_{l=2}^{n} \lambda_l \sum_{i=1}^{k} (\mu_i^l)^2 - \beta nk\end{aligned}$$

The condition $\boldsymbol{\tau}_i \perp \boldsymbol{\tau}_j$ now becomes $\mu_i \perp \mu_j$, while the condition $\|\boldsymbol{\tau}_i\| = 1$ becomes $\|\mu_i\| = 1$. Since the μ_i can be extended to an orthonormal basis matrix M for which M^{T} is also orthonormal, we have

$$\nu_l^2 = \sum_{i=1}^{k} (\mu_i^l)^2 \leq 1$$

with $\sum_{l=1}^{n} \nu_l^2 = k$. Hence, the minimum will occur when $\nu_l^2 = 1$ for $l = 2, ..., k + 1$ and $\nu_l^2 = 0$ for $l > k + 1$. This can be achieved by taking $\mu_i^{i+1} = 1$, $\mu_i^j = 0$, $j \neq i + 1$, or $\boldsymbol{\tau}_i = \boldsymbol{e}^{i+1}$, $i = 1, ..., k$, as stated in the theorem. Note that the minimum energy is

$$\sum_{l=2}^{k+1} \lambda_l - \beta nk$$

If $\lambda_{k+2} > \lambda_{k+1}$, then we must have $\nu_l^2 = 0$ for $l > k + 1$ for the minimum to be achieved. This implies that $\mu_1, ..., \mu_k$ span the same space as $\boldsymbol{e}^2, ..., \boldsymbol{e}^{k+1}$ and can be obtained by an orthogonal transformation of these vectors. Hence the optimal embedding is unique up to orthogonal transformation in R^k. ■

4. APPLICATIONS AND FURTHER RESULTS

We begin by addressing the problem touched on in the Introduction concerning the possibility of solving a problem for which the underlying graph has negative weights.

Theorem 4.1. *Let G be a connected n-vertex weighted graph with some negative weights and adjacency matrix A. The graph drawing problem given in problem 3.1 is solved by taking the weighted graph with adjacency matrix B with off-diagonal entries*

$$B_{uv} = \begin{cases} (A_{uv} + \alpha + \beta) & \text{if } (u,v) \in E(G) \\ \alpha & \text{otherwise} \end{cases}$$

where $\alpha = -\min\{A_{uv} | (u,v) \in E(G)\} > 0$, and computing the eigenvectors $\boldsymbol{e}^1, \boldsymbol{e}^2, ..., \boldsymbol{e}^n$ with corresponding eigenvalues $0 = \lambda_1 < \lambda_2 \leq ... \leq \lambda_n$ of the Laplacian matrix $Q(B)$. An optimal embedding τ is given by $\boldsymbol{\tau}_i = \boldsymbol{e}^{i+1}$, $i = 1, ..., k$ and the minimal value of $E(\tau)$ is

$$\sum_{l=2}^{k+1} \lambda_l - \beta nk - \alpha k$$

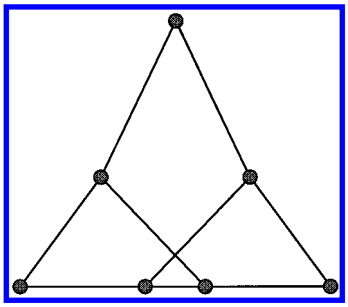

Figure 1. Planar graph drawn with a crossing edge.

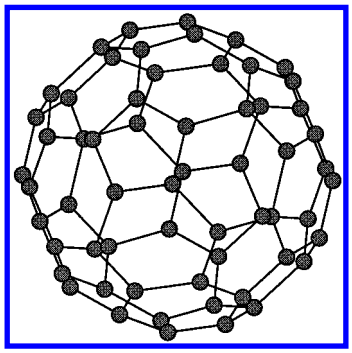

Figure 2. The buckminsterfullerene. The coordinates are determined by the second, third, and fourth eigenvectors.

If $\lambda_{k+1} < \lambda_{k+2}$*, then the optimal embedding is unique up to orthogonal transformations in* R^k.

Proof: The theorem follows from theorem 3.1 and the observation that

$$E_{A+\alpha(J-I)}(\tau) = E_A(\tau) + \alpha k$$

which follows from the computations performed in the proof of theorem 3.1. Hence, a minimum embedding for A is also a minimum embedding for $A + \alpha(J - I)$, while the minimal value of $E(\tau)$ is αk less. ■

Hence the procedure can also be used to find optimal embeddings of graphs with negative weights as might occur in chemical bonds with different repelling strengths.

A question which might naturally arise when considering a novel embedding strategy is whether it is guaranteed to produce a two-dimensional drawing with no crossing edges when presented with a planar graph. For the algorithm of theorem 3.1, this turns out not to be the case as the simple counterexample in Figure 1 shows. The graph is C_7 (the cycle on seven vertices) with two extra edges, (1,5) and (3,7). The graph is clearly planar, but Figure 1 shows the result of applying the algorithm of theorem 3.1.

A good example of the kind of image generated by our method is given in Figure 2, which is the embedding generated for the buckminsterfullerene in R^3 using the second, third, and fourth eigenvectors and taking a two-dimensional projection.

In our definition of the graph drawing task (see problem 3.1), we require that the drawing has normalized variance along the coordinate axes and that the projections onto the coordinates are orthogonal. Together these constraints imply that the drawing will have spherical symmetry in terms of its variance along any axis, since along a (normalized)

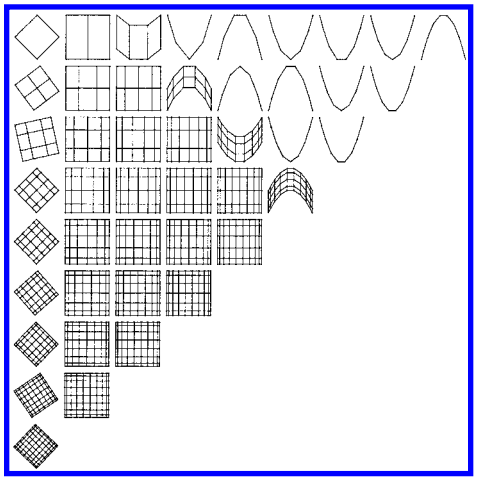

Figure 3. The Cartesian product of two paths $P_n \times P_m$, $2 \le n \le m \le 10$, where the coordinates are given by the second and third eigenvectors of the Laplacian matrix.

direction $\boldsymbol{y} = (y_1, ..., y_k)$ the variance is

$$\|\sum_{i=1}^{k} y_i \boldsymbol{\tau}_i\|^2 = \sum_{i=1}^{k} y_i^2 \|\boldsymbol{\tau}_i\|^2$$

$$= \sum_{i=1}^{k} y_i^2 = 1$$

Hence, in a certain sense we are forcing the graph to "look spherical". For graphs with a naturally eccentric shape our method can break down. In order to illustrate this effect, Figure 3 shows how the method draws the Cartesian product of two paths $P_n \times P_m$, $2 \le n \le m \le 10$ in R^2. The rows of the figure are indexed by n, while the columns are indexed by $m - n$. Hence the leftmost column contains drawings of $P_n \times P_n$, for $n = 2, ..., 10$, while the top row contains the drawings of $P_2 \times P_m$, for $m = 2, ..., 10$.

Note that the figures become degenerate when the difference between m and n is too large and both the second and third eigenvalues are inherited from P_m, causing each copy of P_n to map to a point. The method fails to work because the second harmonic in the longer direction corresponds to a lower Laplacian eigenvalue than the first harmonic in the orthogonal direction. If equality of these two eigenvalues occurs, then a mixture of the two "modes" appears in one coordinate, otherwise the second coordinate becomes a quadratic function of the first and the graph drawing collapses to a line.

In order to show that this problem is not only confined to simple "two-dimensional" graphs, we include a fullerene graph drawn using our technique, which also possesses a degenerate image (see Figure 4). The graph shown is taken from ref 8. Although not immediately apparent from the figure, the three-dimensional coordinates of the vertices all lie on a parabolic (two-dimensional) surface, though in this case no pair of vertices is actually given the same coordinates. This explains why in this case a better image is created by taking the second, fourth, and fifth eigenvectors,[8,9] since the third eigenvector is a harmonic of the second.

We conclude this section by presenting a solution to the second graph drawing problem 3.2, which to a certain extent overcomes the enforced symmetry implicit in problem 3.1.

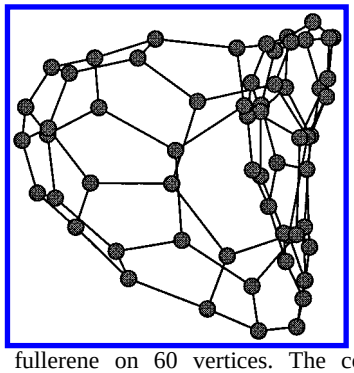

Figure 4. A fullerene on 60 vertices. The coordinates are determined by the second, third, and fourth eigenvectors.

Theorem 4.2. *Let G be a connected n-vertex weighted graph with adjacency matrix A. The graph drawing problem given in problem 3.2 is solved by taking the weighted graph with adjacency matrix B with entries*

$$B_{uv} = \begin{cases} (A_{uv} + \beta) & \text{if } (u,v) \in E(G) \\ 0 & \text{otherwise} \end{cases}$$

and computing the eigenvectors $\boldsymbol{e}^1, \boldsymbol{e}^2, ..., \boldsymbol{e}^n$ *with corresponding eigenvalues* $0 = \lambda_1 < \lambda_2 \leq ... \leq \lambda_n$ *of the Laplacian matrix Q(B). An optimal embedding* τ *is given by*

$$\boldsymbol{\tau}_i = \frac{1}{\sqrt{\lambda_{i+1} - \beta n}} \boldsymbol{e}^{i+1}, \quad i = 1, ..., k$$

Proof: Using the analysis of Theorem 3.1 we can write

$$E(\boldsymbol{\tau}_i) = \sum_{l=2}^{n} (\lambda_l - \beta n)(\mu_i^l)^2$$

where

$$\boldsymbol{\tau}_i = \sum_{l=2}^{n} \mu_i^l \boldsymbol{e}^l$$

and

$$\sum_{i=1}^{k} ||\boldsymbol{\tau}_i||^2 = \sum_{l=2}^{n} \sum_{i=1}^{k} (\mu_i^l)^2$$

By the observation after the definition of problem 3.2, the solution will be invariant to orthogonal rotations. We may therefore assume that the $\boldsymbol{\tau}_i$ are aligned with the eigenvectors $\boldsymbol{e}^{i+1}$ when projected into the subspace spanned by $\boldsymbol{e}^2, ..., \boldsymbol{e}^{k+1}$. Hence, $\mu_i^j = 0$, for $j \neq i + 1$, $j \leq k + 1$. It is now clear that

$$\sum_{i=1}^{k} ||\boldsymbol{\tau}_i||^2$$

is maximized by also taking $\mu_i^j = 0$, for $j > k + 1$, since the norm will have to be smaller in order to have $E(\boldsymbol{\tau}_i) = 1$, after multiplying by larger eigenvalues. Hence, the optimal solution is given by taking $\boldsymbol{\tau}_i = c_i \boldsymbol{e}^{i+1}$. But then

$$E(\boldsymbol{\tau}_i) = (\lambda_{i+1} - \beta n) c_i^2 = 1$$

$$\Rightarrow c_i = \frac{1}{\sqrt{\lambda_{i+1} - \beta n}}$$

as required. ■

The algorithm that is proposed in theorem 4.2 has already been adopted by Manopoulos and Fowler[8] with improved results for less symmetrical graphs than the algorithm of theorem 3.1.

If we apply the MDS method of Kruskal and Seery[6] to a graph which is vertex transitive (i.e., has a group of automorphisms which acts transitively on the vertices, ensuring the graph "looks the same" from the viewpoint of any vertex), the result will be that $\boldsymbol{\tau}_i$ is set to a different but related multiple of $\boldsymbol{e}^{i+1}$. This follows from the fact that the MDS method acts as a uniform procedure in this case together with the fact that the eigenvectors of the adjacency matrix of a regular graph coincide with those of its Laplacian matrix.

5. CONCLUSIONS

We have presented an analysis characterizing two graph drawing procedures that have been adopted by different researchers, principally for drawing fullerene molecules. The characterization is pleasing in itself, but also throws light on the performance of the procedures and in particular clarifies when they are likely to perform well.

It is not clear how the results might be generalized if the norms used are altered, either in the energy function or in the accompanying constraints on the vectors $\boldsymbol{\tau}_i$. It is likely that an analytical solution will not be possible in this case.

A question that remains unresolved in our understanding of the application of these methods is a satisfactory way of determining when the eigenvectors for the smallest eigenvalues are harmonics of those already used and should therefore be discarded. Those using the methods have derived various heuristics, but it would be useful to gain greater understanding of the factors involved.

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