

# Characterising Graph Drawing with Eigenvectors\*

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## 1 Introduction

We consider the problem of embedding a graph on  $n$  vertices in Euclidean space  $\mathcal{R}^k$ , for  $k < n$ . Typically  $k$  would be 3 or 2. By posing the problem as minimising the squared norm of the appropriately weighted distance between adjacent points subject to natural normalising 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 non-adjacent vertices. In this case and for regular graphs the technique has been applied by Pisanski [4], 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 [3].

For distance-regular graphs with a second eigenvalue of multiplicity at least  $k$  the embedding has interesting properties; see Godsil [2].

This paper demonstrates that a problem, that has been traditionally solved by gradient descent techniques used to minimise a measure of poverty of the generated embedding, affords an analytical solution which can be

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implemented in an efficient deterministic algorithm [4]. 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 [5, 6]. The approach presented here is related but corresponds to solving the equation without boundary conditions. The characterisation in terms of minimising 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].

## 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 iff  $a_{uv} > 0$ . For non-adjacent vertices  $a_{uv} = 0$ . Let the diagonal matrix  $D$  be given by

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

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

We summarise a few known results involving the Laplacian matrix. We will number the eigenvalues of  $Q(G)$  given in ascending order:  $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ , with corresponding eigenvectors  $\mathbf{j} = \mathbf{e}^1, \mathbf{e}^2, \dots, \mathbf{e}^n$ , where  $\mathbf{j}$  is the all one vector, while  $0 < \lambda_2$  if the graph is connected. In addition for any  $n$ -dimensional real vector  $\mathbf{x}$  it can be verified that

$$\mathbf{x}^T Q(G) \mathbf{x} = \sum_{(u,v) \in E(G)} a_{uv} (\mathbf{x}_u - \mathbf{x}_v)^2. \quad (1)$$

## 3 Graph Drawing Problem

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

$$\tau : V(G) \longrightarrow \mathcal{R}^k.$$

We will place constraints on this mapping in order to ensure that the representation is natural and hopefully pleasing. We will denote by  $\tau_i$  the  $n$ -dimensional vector formed by taking the  $i$ -th coordinate of  $\tau(u)$  for all  $u \in V(G)$ . Thus  $\tau_i$  is an  $n$ -dimensional vector indexed by the vertices of the

graph  $G$ . Our first requirement is that the centre of gravity of the representation is at the origin. This implies that the vectors  $\tau_i$  have average entry 0, or  $\tau_i \perp \mathbf{j}$ , for  $i = 1, \dots, k$ . The next constraint is that the scaling in all dimensions be similar. This is ensured by requiring that

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

Finally we would like the embedding to retain maximum information about the graph. An example of how information can be lost is given when  $\tau_i = \tau_j$  for some  $i \neq j$ , i.e.  $\tau_i$  and  $\tau_j$  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.  $\tau_i \perp \tau_j$ , 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 require non-adjacent vertices to be far apart. Our definition of the graph drawing problem may therefore be stated as follows.

**Problem 3.1** *Graph Drawing of a graph  $G$  given by (weighted) adjacency matrix  $A$  in  $\mathcal{R}^k$ .*

Find a mapping  $\tau : V(G) \rightarrow \mathcal{R}^k$ , which minimises the following energy function

$$E(\tau) = \sum_{(u,v) \in E(G)} a_{uv} \|\tau(u) - \tau(v)\|_2^2 - \beta \sum_{(u,v) \notin E(G)} \|\tau(u) - \tau(v)\|_2^2,$$

subject to the constraints

$$\begin{aligned} \|\tau_i\| &= 1, & \tau_i \perp \mathbf{j}, & \text{ for } i = 1, \dots, k \\ \tau_i &\perp \tau_j, & \text{ for } 1 \leq i < j \leq k, \end{aligned}$$

where  $\beta$  is a positive constant controlling the strength of the force driving non-adjacent vertices apart. ■

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

**Theorem 3.1** *Let  $G$  be a connected 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*

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

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

$$\sum_{\ell=2}^{k+1} \lambda_\ell + \beta nk.$$

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

**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  $\beta$ .*

**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  $\beta$ . ■

## 4 Proof of Result

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

$$E(\tau) = \sum_{(u,v) \in E(G)} (a_{uv} + \beta) \|\tau(u) - \tau(v)\|_2^2 - \beta \sum_{(u,v) \in E(K_n)} \|\tau(u) - \tau(v)\|_2^2, \quad (2)$$

where  $K_n$  is the complete graph on the vertices of  $G$ . If we consider the complete graph in equation (1), the following equality is obtained for an  $n$  dimensional real vector  $\mathbf{x}$ .

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

In general we have the following relation for an embedding  $\tau$  and graph  $G$  with adjacency matrix  $A$  and Laplacian matrix  $Q$ .

$$\sum_{(u,v) \in E(G)} a_{uv} \|\tau(u) - \tau(v)\|_2^2$$

$$\begin{aligned}
&= \sum_{(u,v) \in E(G)} a_{uv} \sum_{i=1}^k (\tau(u)_i - \tau(v)_i)^2 \\
&= \sum_{i=1}^k \sum_{(u,v) \in E(G)} a_{uv} (\tau(u)_i - \tau(v)_i)^2 \\
&= \sum_{i=1}^k \tau_i^T Q \tau_i,
\end{aligned} \tag{4}$$

by equation (1). Combining the results of equations (2), (3) and (4), we obtain the following expression for the energy function  $E(\tau)$ .

$$E(\tau) = \sum_{i=1}^k \tau_i^T [Q(B) - \beta(nI - J)] \tau_i \tag{5}$$

Let  $\mathbf{j} = \mathbf{e}^1, \dots, \mathbf{e}^n$  be the eigenvectors of  $Q(B)$  with corresponding eigenvalues  $0 = \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n$  and assume that  $\|\mathbf{e}^i\| = 1$  for  $i > 1$ . We have

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

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

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

Hence the eigenvectors of  $Q(B)$  are also eigenvectors of  $Q(B) + \beta(nI - J)$ . Expressing  $\tau_i$  in the eigen-basis, we have

$$\tau_i = \sum_{\ell=2}^n \mu_i^\ell \mathbf{e}^\ell,$$

where  $\mu_i^1 = 0$  since  $\tau_i \perp \mathbf{j} = \mathbf{e}^1$ . Hence we can write the energy of  $\tau$  as

$$\begin{aligned}
E(\tau) &= \sum_{i=1}^k \sum_{\ell=2}^n (\mu_i^\ell)^2 \lambda_\ell \\
&= \sum_{\ell=2}^n \lambda_\ell \sum_{i=1}^k (\mu_i^\ell)^2.
\end{aligned}$$

The condition  $\tau_i \perp \tau_j$  now becomes  $\mu_i \perp \mu_j$ , while the condition  $\|\tau_i\| = 1$  becomes  $\|\mu_i\| = 1$ . Since the  $\mu_i$  can be extended to an orthonormal basis

matrix  $M$  for which  $M^T$  is also orthonormal we have

$$\nu_\ell^2 = \sum_{i=1}^k (\mu_i^\ell)^2 \leq 1$$

with  $\sum_{\ell=1}^n \nu_\ell^2 = k$ . Hence, the minimum will occur when  $\nu_\ell^2 = 1$  for  $\ell = 2, \dots, k+1$  and  $\nu_\ell^2 = 0$ , for  $\ell > k+1$ . This can be achieved by taking  $\mu_i^{i+1} = 1$  or  $\tau_i = \mathbf{e}^{i+1}$ , as stated in the theorem. Note that the minimum energy is

$$\sum_{\ell=2}^{k+1} \lambda_\ell + \beta nk.$$

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

## 5 Conclusions

In our requirements on the embedding we are forcing the graph to “look spherical”. For graphs with natural excentric shape our method does not give natural pictures. This problem may also explain why occasionally a better image is created by taking the 2nd, 4th and 5th eigenvectors, [3], [4], rather than the three eigenvectors corresponding to the three smallest non-zero eigenvalues. The following figure shows how our method draws the Cartesian product of two paths  $P_n \times P_m, 2 \leq n \leq m \leq 10$ . The fullerene graph on figure 3 is taken from [3].

We have not considered the case where edges are allowed to have negative weights. We have seen, however, that adding multiples of the matrix  $J - I$  does not affect the eigenvectors of the Laplacian matrix, though corresponding eigenvalues are increased. Hence we can add a multiple of  $J - I$  to a graph with negative weights in order to create one with only positive ones. This will shift the energy function by a fixed amount and so the optimal embeddings of the two graphs will coincide, though the minimal value of the energy function will of course change. 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.

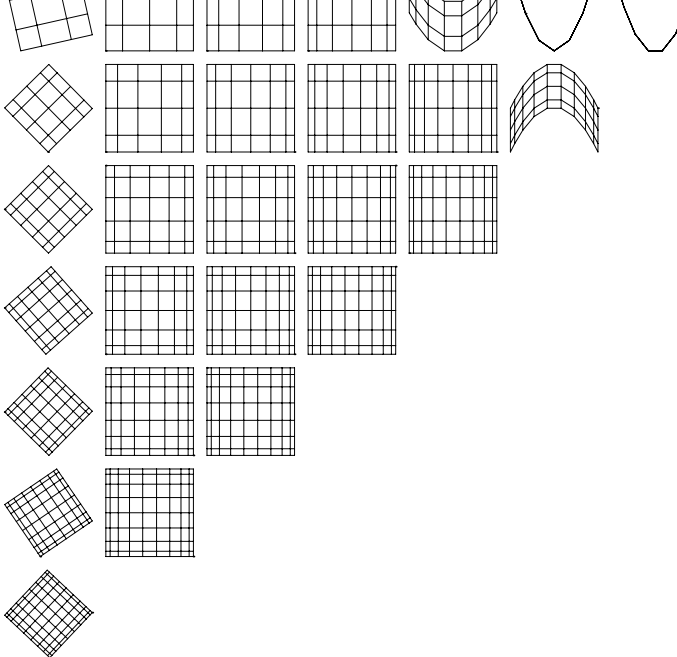


Figure 1: The Cartesian product of two paths  $P_n \times P_m$ ,  $2 \leq n \leq m \leq 10$ , where the coordinates are given by the second and third eigenvector of the Laplacian matrix.

It is not clear how the results might be generalised if the norms used are altered, either in the energy function or the accompanying constraints on the vectors  $\tau_i$ . It may well be that in this case the approach taken in this paper is not applicable and a more standard method of energy minimisation must be applied.

## References

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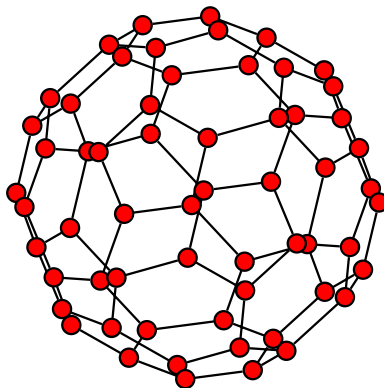


Figure 2: The Buckminster fullerene. The coordinates are determined by the 2nd, 3rd and 4th eigenvector.

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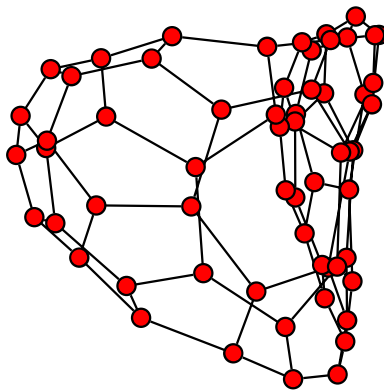


Figure 3: A fullerene on 60 vertices. The coordinates are determined by the 2nd, 3rd and 4th eigenvector.