Partitioning Networks by Eigenvectors

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Abstract

A survey of published methods for partitioning sparse arrays is presented. These include early attempts to describe the partitioning properties of eigenvectors of the adjacency matrix. More direct methods of partitioning are developed by introducing the Laplacian of the adjacency matrix via the directed (signed) edge-vertex incidence matrix. It is shown that the Laplacian solves the minimization of total length of connections between adjacent nodes, which induces clustering of connected nodes by partitioning the underlying graph. Another matrix derived from the adjacency matrix is also introduced via the unsigned edge-vertex matrix. This (the Normal) matrix is not symmetric, and it also is shown to solve the minimization of total length in its own non-Euclidean metric. In this case partitions are induced by clustering the connected nodes. The Normal matrix is closely related to Correspondence Analysis.

The problem of colouring graphs (which is in a sense dual to the problem of clustering induced by minimizing total distances) is also considered. A heuristic method to produce approximate correct colourings using sign patterns of eigenvectors with large negative eigenvalues is described. The formulation used to solve the minimization problem may also be used to solve the maximization problem, which leads to approximate colourings from both the Laplacian and the Normal matrix.

Introduction

There has been a recent renewal of interest in spectral methods for partitioning large sparse arrays, based on results that first appeared in the literature over twenty years ago. Hagen (1992) speculates that this is because growth in problem complexity has exposed scaling weaknesses in iterative methods such as Kernighan and Lin (1970), Kirkpatrick, *et al*., (1983), where problems now include finding efficient methods for distributing large adaptive finite mesh problems to arrays of parallel processors. The methods currently being developed exploit global properties of the underlying graph representation of the sparse array and so should be of interest to Social Network researchers. We present a brief survey of some early attempts to understand

network structure from the Standard[1] spectral representation and introduce the Laplacian spectrum as a method for obtaining useful results more directly. We also introduce another spectral representation (called Normal, because its spectral radius is always 1), show that it shares some desirable properties with the Laplacian, and suggest that it provides a useful model for obtaining important global properties from social and other sparse networks.

The Standard Spectrum

(Gould, 1967) provides an introduction to the linear algebra of eigendecomposition of connection (adjacency) matrices as applied to networks of roads, and uses the components of the Frobenius eigenvector (the eigenvector belonging to the most positive eigenvalue) to assign values of "accessability" to the nodes of the network. He gives an example of the road networks of Uganda and attempts less successfully to interpret the meanings of other eigenvectors in terms of "peripherality" and "inner-connectedness". The interpretation of negative[2] eigenvectors is simplified away by weighting the diagonal, thus reducing their importance. Tinkler (1972) extends this analysis with some discussion of the connection matrix as a transition probability matrix, and of the meanings of eigenvectors from a communication point of view (e.g. "rumors and anti-rumors") as measuring a diffusion process. Difficulties in interpreting the partitions induced by the second and other eigenvectors (in a physical sense) leads to an attempt to provide more useful partitions via Factor Analysis.

The problem of using Standard eigenvectors to provide useful partitions is examined in papers by Donath and Hoffman (1973) and Barnes (1982), both of which depart from the Standard spectrum. Barnes uses a Linear Programming technique based on the transportation problem to find partitions with the minimum number of connections between them. The technique is interesting since it uses both first and second positive eigenvectors to find a 2-way partition, the first three to find a 3-way partition, and the method can evidently be extended. The former considers the more general problem of finding n-way partitions *directly* by weighting the diagonal of the connection matrix.

This approach is crucial in the algorithm developed by Hall (1970), which we describe in detail. He considers the problem of finding the *minimum* z of the weighted sum

$$z = 1/2 \sum_{i,j} (x_i - x_j)^2 a_{ij} \qquad \textbf{(1)}$$

where a_{ij} are the elements of the adjacency matrix A. The sum is over all pairs of squared distances between nodes *which are connected*, and so the solution should result in nodes with large numbers of inter-connections being clustered together[3].

Equation 1 can be re-written as:

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[1] We use the term "Standard" to refer to the eigendecomposition of the *adjacency matrix* of a graph: the standard method in algebraic graph theory.

[2] The terms "negative", "positive", "largest", etc. are used to refer to the eigenvector with eigenvalues of those signs and/or magnitudes.

[3] More recent papers such as (Walshaw et al, 1995) derive this result explicitly in terms of minimizing the number of edges between subsets, thus emphasizing the partitioning properties of the solution.

$$1/2 \sum_{i,j} (x_i^2 - 2x_{ix_j} + x_j^2) a_{ij} = 1/2 \sum_i x_i^2 a_{i\bullet} - 2 \sum_{i,j} x_i x_j a_{ij} + \sum_j x_j^2 a_{\bullet j} =$$

$$\sum_i x_i^2 a_{i\bullet} + \sum_i \sum_{j \neq i} x_i x_j a_{ij} = X^t B X$$

where $B = D - A$ is referred to as the "disconnection matrix", and $D = Diag\ (\sum_i a_{ij})$.

In addition to this, Hall supplies the condition that $X^t X = 1$, i.e., the distances are measured in the Euclidean metric. Using Lagrange multipliers, we have:

$$z = X^t B X - \lambda X^t X$$

and taking derivatives with respect to X gives:

$$B X - \lambda X = 0 \quad \text{or} \quad B X = \lambda X \qquad (2)$$

which is an eigenvalue problem.

Hall goes on to solve this problem in a number of dimensions (each eigenvector supplies a new dimension), and makes the very interesting observation that (2) may also be considered as a *maximization* problem. That is, the eigenvector associated with the largest solution to (2) maximizes the total distance between connected nodes, and so should provide a partition with a large number of edge crossings, and clusters with *few* connections among the nodes. Such a partition should provide an approximate correct *colouring*.

The problem of finding correct colourings of a graph is, in a sense, dual to that of finding partitions which minimize distance between connected nodes. Aspvall and Gilbert (1984) present a heuristic for colouring graphs based on the most *negative* eigenvectors. This heuristic is shown to provide the minimum correct colouring for a class of graphs called *block regular* (for example, cocktail party graphs of order n can always be given minimum correct colourings by considering the sign patterns of the $n-1$ most negative eigenvectors). Their paper suggests that the sign patterns of *only* the most negative eigenvectors will always give a correct colouring (including the trivial colouring, in which each node is given a distinct colour). This is certainly true if *all* eigenvectors are considered, but remains a conjecture if *only* the negative eigenvectors are considered.

It is evident that the Standard spectrum - though it has many useful applications in Algebraic Graph Theory (especially for regular graphs) - requires that we *either* form combinations of its eigenvectors to apply it to problems such as clustering and partitioning (and thus overcome "leakage" of useful information into the family of eigenvectors), *or* devise better "filters" by deriving new matrices from the Standard adjacency matrix. We explore the latter approach, and look at two particular cases:

Additive: $(D+A)X = \lambda X$ and **Multiplicative:** $(DA)X = \lambda X$,

where D is some diagonal matrix. Conditions under which solutions to these problems exist (easily satisfied in the cases we consider) may be found in Freidland (1977) and Biegler-König (1981).[4]

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[4]In a series of papers, (e.g. Borgatti and Everett 1992) based a theory of structural equivalence on various forms of graph colourings. We will examine both cases for their ability to providing useful colouring partitions as well.

The Laplacian Spectrum

We introduce the Laplacian of a graph by defining the *signed edge-vertex incidence matrix* (Biggs, 1974) as follows: For a graph $G(V,E)$ form a matrix Δ with $|V|$ rows and $|E|$ columns, where

$$\delta_{ij} = \begin{cases} +1 \text{ if } v_i \text{ is the positive end of } e_j \\ -1 \text{ if } v_i \text{ is the negative end of } e_j \\ 0 \text{ otherwise} \end{cases}$$

Obviously for a symmetric graph there is some arbitrariness in assigning signs to the row elements, but this can be ignored here as long as each column contains exactly one +1 and one -1. The matrix Δ defines a set of *first-differences* between the nodes of G, and may be thought of as the discrete analogue of the continuous *gradient operator* ∇. The square[5] $\Delta\Delta^T$ may be thought of as the discrete analogue of the continuous Laplacian operator ∇^2, and this matrix L is simply the "disconnection" matrix B defined above:

$$L = B = D - A$$

Although this additive variation of the adjacency matrix may seem like a very simple one, a large literature has developed on the Laplacian in the last 10 years, mainly because this discrete analogue shares so many important properties with its continuous version, undoubtedly the most important and best understood operator in mathematical physics[6]. It first appears in (Kirchoff, 1847) where it is called the "admittance matrix". Some useful discussions of its properties are found in [1, 2, 3, 9, 13, 16, 18, 21, 22]. Mohar (1991) presents a convincing case for considering the Laplacian as being a more fundamental matrix than the adjacency matrix for algebraic graph theory. Discussions of practical use in partitioning large sparse matrices are found in [5, 23, 33, 35, 37]. Because of the discussion in Fiedler (1975), the eigenvector belonging to the *second-smallest* eigenvalue of L has been called the Fiedler eigenvector.

We note one important property of the Laplacian spectrum as discussed in Pothen *et al.* (1990): the relationship between the Fiedler eigenvalue and the *isoperimetric number* (Alon, 1986) which is related to the problem of computing good edge separators. It appears that the clustering solution found by Hall (1970) results from a side-effect of this property: the Laplacian produces partitions, which indirectly produces clusters (we shall see this more clearly when we consider graph coloring).

The Frobenius eigenvector of the adjacency matrix of a regular graph always has constant components, but this is not the case for non-regular graphs. However, for the Laplacian we can immediately see (since all the rows sum to zero) that there *is* always an eigenvector with constant components, and that its eigenvalue is zero. Further, since L is positive semi-definite, all other eigenvalues must be greater than zero for a connected graph. If a graph is *not* connected, then the multiplicity of eigenvalue 0 must equal the number of

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Research into these matters is still incomplete.

[5]We will not consider the "other" square $\Delta^T\Delta$, except to note that it is closely related to the line graph of G. For this square, the assignment of signs is important (Biggs, 1974).

[6] The analogy is exact when Neumann boundary conditions are imposed (Freidman, 1993).

disconnected components. Thus an eigenvalue *near* zero must belong to an eigenvector with both positive and negative components which partition the graph into "nearly" disconnected components.

With this observation we can continue in two possible directions: a) Use the Fiedler eigenvector to partition the graph into subgraphs, find the Fiedler eigenvector of each sub-graph, and continue recursively until the sub-graphs all satisfy some maximum size criterion. This approach is called Recursive Spectral Bisection (RSB) [5, 35, 37] and has been used very successfully on adaptive mesh problems for parallel processors. RSB is similar in approach to the CONCOR heuristic for finding blocks in a network (Brieger, *et al.*, 1975). b) Use the third-smallest, fourth smallest, etc. eigenvectors to induce further partitions, and thus induce clusters of nodes. This is similar to other MDS methods for finding block (or group) structure in networks (Barnett, 1993; Seary & Richards, 1995).

While the Laplacian spectrum has many attractive theoretical properties which make it very useful for partitioning large sparse arrays, it has at least one drawback: the Fiedler eigenvector is associated with the *second smallest* eigenvalue. The current method of choice for finding a few eigenvectors of very large sparse matrices is the Lanczos method, which tends not to find small eigenvectors as quickly as it finds the *largest* eigenvectors (Pothen, et al, 1990). Another drawback with the Laplacian is application to the colouring problem. The Laplacian does not have negative eigenvalues, but the observation of Hall (1970) suggests that the *largest* eigenvector will partition the graph such that connected nodes will be as far apart as possible. However, when forming colourings based on sign patterns, it is difficult to determine where to stop.

The Normal Spectrum

The Laplacian is based on a second-differences matrix. We now introduce a matrix based on *averages*, starting with the *unsigned* edge-vertex incidence matrix. We average by dividing each row by the square root of its row sum, and each column by the square root of its column sum. (Note that each column adds to exactly two, so this amounts to a constant scaling of the columns). Squaring[7] this yields:

$$D_R^{-1}(A+D)\,D_C^{-1} \qquad (3)$$

Equation **3** looks like a mixture of additive and multiplicative eigenvalue problems, until we realize that $\boldsymbol{D_C}$ is really a constant multiplier and can be ignored, and

$$D_R^{-1}(A+D) = M+I$$

where $M=D_R^{-1}A$ and $\boldsymbol{I}$ is an identity matrix of appropriate size. In fact, since $\boldsymbol{I}$ is an identity matrix, we can form linear combinations of $\boldsymbol{M}$ and $\boldsymbol{I}$ (and their eigenvalues) without changing the resulting eigenvectors. In general, we can write:

$$(dI+(1-d)\,M)\,X = \lambda X \qquad (4)$$

as a *family* of eigenvalue equations. We examine this in more detail later for values of $\boldsymbol{d = 0}$ and $\boldsymbol{0.5}$.

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[7] Again, we do not consider the "other" square, except to note that here the assignment of signs is not important, unlike the Laplacian case. It is less closely related to the line graph of G.

Just as with the Laplacian, we can immediately deduce one eigenvalue and associated eigenvector for ***M***, since: a) All elements of ***M*** are non-negative; and b) All rows of ***M*** sum to ***1***. This means that ***M*** is a stochastic matrix, and that it has an eigenvalue of ***1*** and an associated eigenvector of constant components. Further, all other[8] eigenvalues are less than ***1*** in absolute value for a connected graph, and we can go on to make the same arguments about the second *largest* eigenvalue of ***M*** that we made for the second *smallest* eigenvalue of ***L***: the multiplicity of an eigenvalue of ***1*** equals the number of disconnected components of the network, and eigenvalues *near* ***1*** are associated with eigenvectors that *partition* the network into *nearly* disconnected parts. In this case we will find that the partitioning properties of ***M*** are indirectly produced by its *clustering* properties.

One way to show the clustering properties of ***M*** is to reproduce the argument of Hall (1970) but with a different definition of distance. We use $z = X^t L X - \zeta X^t D_R X$

$$X^t D_R X = 1 \tag{5}$$

as a metric and so the Lagrange expression becomes $z = X^t L X - \zeta X^t D_R X$ and the associated eigenvalue problem is $LX = \zeta D_R X$ or:

$$(I - M)X = \zeta X \tag{6}$$

As in the Euclidean case, there is a trivial solution of $\zeta_0 = 0$ and $x_i = x_j$ and other one-, two-, etc. dimensional solutions for $0 < \zeta_1 \leq \zeta_2 \ldots$ where ζ_j is related to μ_j, the corresponding eigenvalue of ***M***, by $\zeta_j = 1 - \mu_j$ where $1 = \mu_0 > \mu_1 \geq \ldots \geq \mu_n \geq -1$.

However, note that the condition **(5)** results in a non-Euclidean metric D_R, so that the eigenvectors are not (in general) orthogonal in Euclidean space, although they are in D_R, space. This is to be expected, since ***M*** is not, in general, symmetric. Note also that $0 = \zeta_0 < \zeta_1 \leq \ldots \leq 2$ since the eigenvalues of ***M*** are always ≤ 1 in absolute value. Finally, note that ζ_n (and the most negative μ) represents the *maximum* solution.

We argued that for ***L***, the clustering was a side-effect of partitioning. We claim that for ***M***, partitioning is a side-effect of clustering. The Normal spectrum has a close association with correspondence analysis (CA). The only differences are that CA weights the Normal eigenvectors by the corresponding eigenvalues (so that CA eigenvectors with small eigenvalues are shorter than Normal eigenvectors, but still have the same directions), and the CA eigenvalues are always positive. We argue that the well-known clustering properties (Nishisato, 1980; Greenacre, 1984) of CA also hold for the Normal eigenvectors. In particular, the property of *Distributional Equivalence*[9] holds.

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[8] It is possible to have more than one eigenvalue of absolute value 1. If the graph is bipartite, there will also be an eigenvalue of -1, and we will deal with this later.

[9] This property allows identical rows and columns to be added (reducing the size of the problem) without changing the Normal spectrum (Greenacre, 1984)

The clustering property holds as well when the eigenvector of $\boldsymbol{M}$ belongs to a *negative* eigenvalue. This property is hidden when CA is used to examine a network, since it always returns the *absolute value* of eigenvalues. For a symmetric network, the sign of an eigenvalue is "hidden" by making the components of the column eigenvectors opposite in sign to the components of the row eigenvectors; for positive eigenvalues, they are identical. For this reason, we prefer to work *directly* with the Normal spectrum, from which the CA spectrum is easily calculated. Negative eigenvalues of $\boldsymbol{M}$ can be avoided by weighting the diagonal of the original adjacency matrix, but the weighting *cannot* be some constant, since this will distort the eigenvectors. As equation 4 shows, it is more straightforward to deal directly with the important eigenvectors of $\boldsymbol{M}$, from which solutions based on "strictly positive" or "mixed" eigenvalues can readily be derived by assigning a value to the "damping factor" $\boldsymbol{d}$. These matters are addressed in some detail in Richards & Seary (1995). Briefly:

a) No damping: $\boldsymbol{d = 0}$ allows the negative (colouring) eigenvectors as much importance as the positive (cohesive) eigenvectors. We have found many social networks have important negative eigenvalues.

b) Critical damping: $\boldsymbol{d = .5}$ guarantees that all eigenvalues are non-negative, so that the important eigenvectors are those that form *cohesive* clusters among *connected* nodes. This models Convergence Theory (Richards & Seary,1995). Note that the eigenvectors themselves do not change, only the relative importance as selected by choosing a value for $\boldsymbol{d}$.[10]

Comparisons of Standard, Laplacian, and Normal Spectra

In this section we compare results of the three methods for some sample networks. For regular graphs of degree $\boldsymbol{d}$, it is easy to show that all three give the same eigenvectors, and the eigenvalues are related as follows:

$$\lambda_j = d - \sigma_j \qquad \mu_j = \sigma_j / d$$

where σ_j, λ_j and μ_j are eigenvalues for Standard, Laplacian, and Normal decomposition. All three have an extreme (largest or smallest) eigenvector with constant components.

For non-regular networks, both Laplacian and Normal decompositions produce an extreme eigenvector with constant components. For the Laplacian, this eigenvector belongs to eigenvalue 0, for the Normal it belongs to eigenvalue 1. As an example of a non-regular network, consider a rectangular 6 x 8 grid (chosen because it is regular enough to show the types of problems that will show up for a *very* irregular network). Figure 1 shows a display of this network with the nodes at coordinates specified by the second and third most extreme positive eigenvectors for each spectrum. All three methods provide a useful partition, but the Laplacian and Normal give a clearer picture of the *topology* of the network.

[10] Other values for d are considered in Yamaguchi (1994).

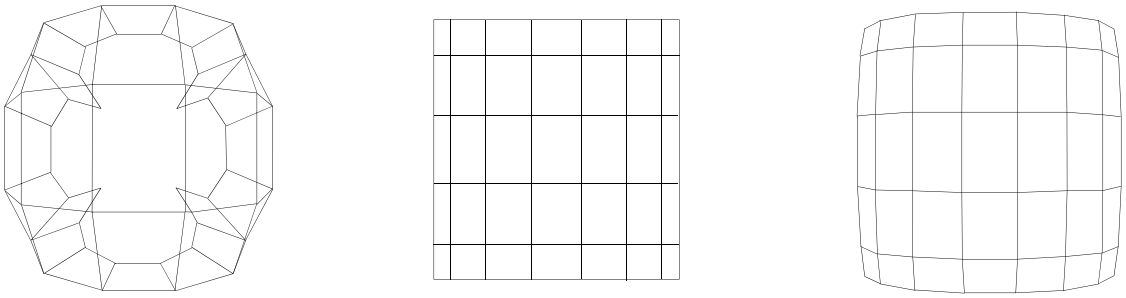


Fig. 1. Standard Laplacian Normal

Figure 2 shows the same network as arranged by the most extreme "negative" eigenvalue[11] (for the Laplacian, the largest). Here both the Laplacian and Standard displays partition the nodes into two groups which have *no* connections between them (the grid is *bipartite* and so may be two-coloured), but the nodes are arranged so that those with fewer connections are nearer the centre. This suggests the problems that will arise for colouring less regular networks. In contrast, the Normal display captures the bipartite-ness perfectly since nodes are *normalized* by the number of connections. This is an example of a partition induced by good clustering, whereas the other two are poor clusters induced by partitioning[12].

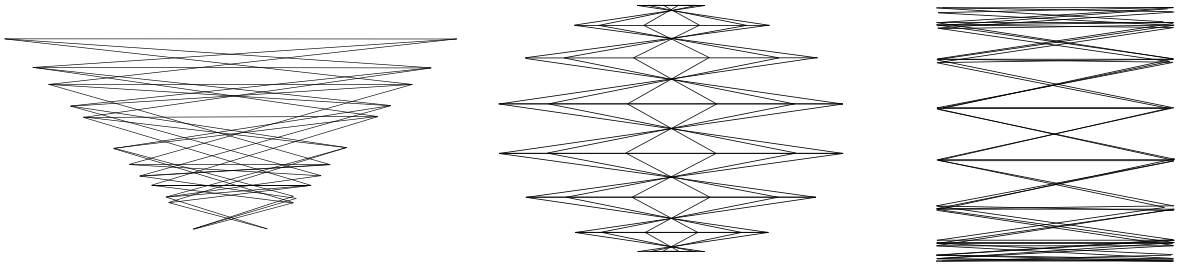


Fig. 2. Standard Laplacian Normal

Figure 3 is an example of a network for which the two largest eigenvectors are both negative. We see that the Standard display shows an approximate colouring as we would expect, but that the Laplacian does not. The Normal display partitions the network into four quadrants representing the four required colours. Figure 3d is the same network displayed using the two most positive Normal eigenvectors, and shows what we would expect to find from a cohesion model.

[11] The displays have been stretched in the y direction to make the patterns clearer.

[12] Note that eigenvalues "near" -1 should induce partitions that produce approximate correct colourings.

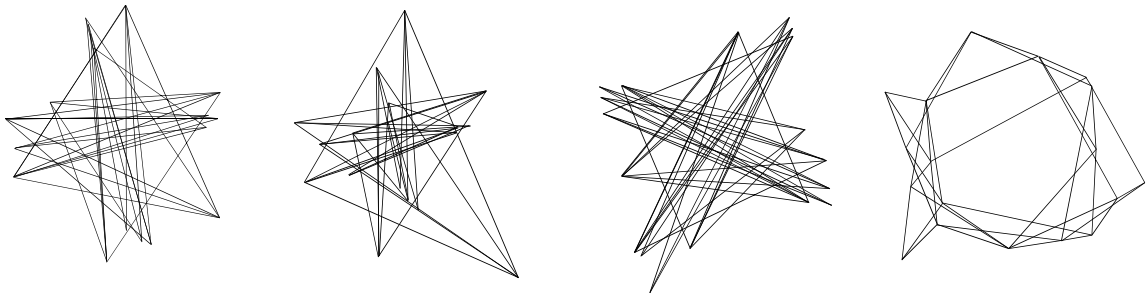


Fig. 3. Standard Laplacian Normal d

Figure 4 shows results for a "mixed" network (common in social networks). The blockmodel for this network can be immediately derived by sorting the adjacency matrix based on sign patterns of the two largest negative *and* positive Normal eigenvectors.

Application and Implementation of the Normal Spectrum

The previous examples suggest that the Normal spectrum is useful as a basis for both *role-based* and *group-based* network analysis. Both signs and magnitudes of its eigenvalues indicate the type and importance of the partitioning induced by the corresponding eigenvectors: eigenvalues near 1 in absolute value measure an important structural eigenvector. Cohesive solutions may be forced by adjusting ***d*** of Equation 4; e.g., for

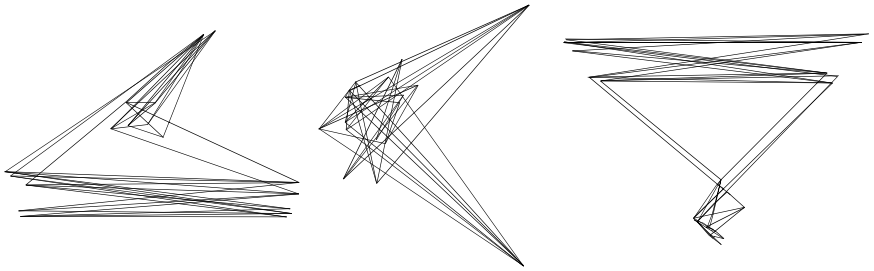
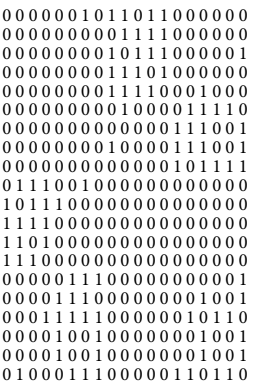


Fig. 4. Standard Laplacian Normal



the regular grid, the coloring solution may be "turned off" simply by choosing ***d = 0.5***, which results in a mesh partition equal to the Laplacian. We have not applied these methods to the large adaptive unstructured meshes discussed in, e.g., [5, 35, 37], but we suggest that the results may be comparable to those of the Laplacian[13], and with somewhat less overhead since the partitions result from the second *largest* eigenvector. Even the lowly Power Method can be used to find a partition!

One apparent problem that must be overcome before Normal decomposition can be used with very large sparse arrays is related to the preferred method for dealing with such arrays: the Lanczos algorithm. This algorithm requires *symmetric* matrices, but matrix ***M*** is asymmetric, even when the original adjacency matrix ***A*** is symmetric. However this problem is easily overcome, since ***M*** is closely related to a symmetric matrix

[13] The small Laplacian and large Normal eigenvectors have large (>.9) correlations, especially when individual vertex degree does not vary much from the average degree. This is often the case for adaptive mesh problems.

$\boldsymbol{T}$ derived from $\boldsymbol{A}$, which fits into the usual Lanczos method without loss of sparsity.

We define $\boldsymbol{T}$ as: $\boldsymbol{T} = \boldsymbol{D}_R^{-1/2} \boldsymbol{A} \boldsymbol{D}_R^{-1/2}$. $\boldsymbol{T}$ is symmetric, has the same eigenvalues as $\boldsymbol{M}$, and its eigenvectors $\boldsymbol{t}_j$ are related to $\boldsymbol{m}_j$, the eigenvectors of $\boldsymbol{M}$, by the relation $\boldsymbol{m}_j = \boldsymbol{D}_R^{-1/2} \boldsymbol{t}_j$.

We now outline how a Lanczos step should proceed[14]:

Initialization:

1) Form vector $R_i = (\sum_j a_{ij})^{-1/2}$ from the row sums of $\boldsymbol{A}$.

2) Form the initial Lanczos vector $v_0(i)$ from $[i-(n+1)/2]R_i$

   (where $[...]$ rounds up for positive and down for negative values) and normalize so that $|v_0| = 1$. This vector is orthogonal to the Frobenius eigenvector of $\boldsymbol{T}$.

Matrix multiplication:

3) The matrix multiplication part of a Lanczos step becomes:

$$u_k(i) = R_i \sum_j a_{ij} v_k(j) R_j$$

   for each Lanczos step $\boldsymbol{k}$. This step can exploit special properties (e.g., sparsity) of $\boldsymbol{A}$.

Termination:

4) When sufficient eigenvectors are found, the exact eigenvectors of $\boldsymbol{M}$ may be computed by multiplying component i of each eigenvector by R_i. This step is unnecessary if the aim is only to find a partition, since R_i is always positive, and so will not change the partition by signs.

[14] Using the notation of (Parlett et al, 1982).

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