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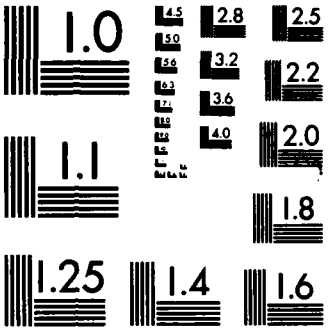

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GRAPH PARTITIONING BY EIGENVECTORS

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1. Introduction

If G is a graph with vertex set $V = \{1,\ldots,n\}$, the adjacency matrix of G is $\mathrm{adj}(G) = A = [a_{ij}]$ with $a_{ij} = 1$ if $\{i,j\}$ is an edge, and $a_{ij} = 0$ otherwise. (Note that $a_{ii} = 0$ for all i.) Conversely if M is a symmetric nonnegative $n \times n$ matrix, the associated graph of M is $G = \mathrm{gr}(M)$ with vertex set $V = \{1,\ldots,n\}$ having as edges all $\{i,j\}$ for which $m_{ij} > 0$ and $i \neq j$. We denote the eigenvalues of A by $\lambda_1(A) \geq \lambda_2(A) \geq \ldots$ and the multiplicity of α in the spectrum of A by $\mathrm{mult}(\alpha:A)$. We may also speak of the eigenvalues and eigenvectors of a graph, meaning those of its adjacency matrix.

The close relationship between graphs and nonnegative symmetric matrices has been exploited to illuminate some matrix concepts. (See Varga, 1962.) If we define the concept of irreducible matrix to include the 1×1 zero matrix, then we have the following (Varga 1962, p. 46).

Theorem A. Let B be a nonnegative symmetric matrix. (1) B is irreducible if and only if $\mathrm{gr}(B)$ is connected. (2) $B = B_1 \oplus \ldots \oplus B_k$ is a direct sum of k irreducible matrices if and only if $\mathrm{gr}(B)$ is a union of k connected components, $G_1,\ldots,G_k$, and $G_i = \mathrm{gr}(B_i)$. □

Recently, some algorithms have been proposed that use the eigenvectors of a graph to partition its vertices in certain ways (Barnes, 1982, Aspvall and Gilbert, 1984). The objective of this paper is to study how the connectivity structure of a graph is revealed by its eigenvectors and its spectrum.

We will freely use familiar properties of matrices such as the extremal nature of eigenvalues of symmetric matrices, the interlacing theorem, monotonicity of spectral radius of nonnegative matrices, Perron-Frobenius theory, etc. (See Varga (1962) and Lancaster and Tismenetsky (1985).)

Most of the results of this paper depend on the following lemma.

ABSTRACT

Let A be the adjacency matrix of a connected graph G. If z is a column vector, we say that a vertex of G is positive, nonnegative, null, etc. if the corresponding entry of z has that property. For z such that $Az \geq \alpha z$, we bound the number of components in the subgraph induced by positive vertices. For eigenvectors z having a null element, we bound the number of components in the graph induced by non-null vertices. Finally, bounds are established for the number of null elements in an eigenvector, for the multiplicity of an eigenvalue and for the magnitudes of the second and last eigenvalues of a general or a bipartite graph.

Lemma. Let B be a principal square submatrix of a real symmetric matrix A, and suppose that $B = B_1 \oplus \ldots \oplus B_k$ where the B_i are irreducible. If $\lambda_1(B_i) \geq \beta$ for $i = 1,\ldots,k$, then $\lambda_k(A) \geq \beta$ also.

Proof. Each eigenvalue of a B_i is an eigenvalue of B. Thus the $\lambda_1(B_i)$ are k eigenvalues of B, each at least as large as β; hence $\lambda_k(B) \geq \beta$. The conclusion follows by the interlacing theorem: $\lambda_k(A) \geq \lambda_k(B)$.

Note that a strict inequality for the $\lambda_1(B_i)$ yields a strict inequality for $\lambda_k(A)$ also. □

2. Fiedler's Theorem

The first step in studying graph structure with eigenvectors was taken by Fiedler (1975). The following is a version of his Theorem 2.1.

Theorem B. Let A be an irreducible nonnegative symmetric nxn matrix, $n \geq 2$, and z be a column such that $Az \geq \alpha z$, $\alpha = \lambda_s(A)$, $s \geq 2$. If

$$z = \begin{bmatrix} x \\ -y \end{bmatrix}, \quad A = \begin{bmatrix} B & C \\ C^T & D \end{bmatrix}$$

with $x \geq 0$, $y > 0$, and if $B = B_1 \oplus \ldots \oplus B_k$ where the B_i are irreducible, then $k < s$. □

In order to rephrase this theorem in terms of graphs, let us define comp(G) to be the number of connected components of a graph G, and, for an n x 1 column z, let

$$P(z) = \{i : z_i > 0\},\ N(z) = \{i : z_i < 0\},\ Z(z) = \{i : z_i = 0\}.$$

When these are interpreted as subsets of a vertex set, we may speak of positive, negative or null vertices. (Dependence on z will be suppressed when no confusion results.) Angle brackets around a set of vertices mean the subgraph induced by that set.

Theorem B'. Let G be a connected graph on $n \geq 2$ vertices, $A = \mathrm{adj}(G)$, and z a column such that $Az \geq \alpha z$, $\alpha = \lambda_s(A)$, $s \geq 2$. Then

$$\mathrm{comp}(\langle P \cup 0 \rangle) \leq \max\{i:\lambda_i(A) > \alpha\}. \quad \square$$

Proof. Suppose vertices numbered so that matrices B, C and x from Theorem B may be partitioned as

$$B = \begin{pmatrix} B_1 & & \\ & \ddots & \\ & & B_k \end{pmatrix} \quad x = \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix} \quad C = \begin{pmatrix} C_1 \\ \vdots \\ C_k \end{pmatrix}$$

where the B_i are irreducible. The hypothesis $Az \geq \alpha z$ implies that $B_i x_i - C_i y \geq \alpha x_i$ for each i. Since A is irreducible, no C_i is 0. Thus $C_i y \geq 0$ with inequality in some element, and hence $B_i x_i \geq \alpha x_i$ with strict inequality in some element. Therefore, for each $i = 1,\ldots,k$,

$$x_i^T B_i x_i > \alpha x_i^T x_i \tag{1}$$

and $\lambda_1(B_i) > \alpha$. From the lemma, $\lambda_k(A) > \alpha$; thus $k \leq \max\{i:\lambda_i(A) > \alpha\}$. $\square$

Several corollaries can be extracted from the proof of the theorem.

Corollary 1. If $\alpha > 0$, then no component of $\langle P \cup 0 \rangle$ (a) is a singleton, or (b) contains vertices only from 0.

Proof. If the ith component were a singleton, its 1×1 adjacency matrix would be $B_i = 0$; but then Eq. (1) would be false. Similarly, if the ith component contained vertices from 0 alone, then x_i would be 0, and again Eq. (1) would be false. $\square$

The other corollary depends on the fact that all connected graphs with spectral radius less than 2 are known (Smith, 1970). The four smallest spectral radii are 0, 1, $\sqrt{2}$, $(1+\sqrt{5})/2$, belonging to the paths on 1, 2, 3 and 4 vertices respectively.

Corollary 2. For α in the indicated range, $\mathrm{comp}(\langle P \cup 0 \rangle)$ does not exceed the upper bounds shown.

	Range	Bound 1	Bound 2
(a)	$\alpha < 0$	$\max\{i:\lambda_i(A) \geq 0\}$	-
(b)	$0 \leq \alpha < 1$	$\max\{i:\lambda_i(A) \geq 1\}$	$(n-1)/2$
(c)	$1 \leq \alpha < \sqrt{2}$	$\max\{i:\lambda_i(A) \geq \sqrt{2}\}$	$(n-1)/3$

Proof: (a) Referring back to the proof of Theorem B, and to Eq. (1), we see that $\lambda_1(B_i) \geq 0$, because each B_i is the adjacency matrix of a connected subgraph of G.

(b) If all the B_i have a positive spectral radius, they must all have spectral radius at least equal to 1. Also, each B_i must have at least two rows, and D has at least one row. Hence the number of the B_i is at most (n-1)/2. A similar argument holds for case (c). More cases could be added, but their significance and usefulness decrease. □

The next theorem indicates the role played by the null vertices in holding together the components of $\langle PUO \rangle$. They affect the bound on the number of components only if α is an eigenvalue of A.

Theorem 1. Let A and z be as in Theorem B'. Then

$$\text{comp}(\langle P \rangle) \leq \max\{i:\lambda_i(A) \geq \alpha\}.$$

Proof. We use the notation of Theorem B and its proof, except that $x > 0$, $y \geq 0$. As before, $B_i x_i - C_i y \geq \alpha x_i$, but now $C_i y$ could be zero, so we have only

$$B_i x_i \geq \alpha x_i \tag{2}$$

for each i. Thus $\lambda_1(B_i) \geq \alpha$, and the conclusion follows from the lemma. □

Note that the proofs of Theorem 1 and Theorem B' make no use of the implied inequality $C^T x - Dy \geq -\alpha y$, which we may thus safely ignore. With this observation it becomes easy to bound the number of components of any induced subgraph of a connected graph.

Theorem 2. Let G be a connected graph, U a proper subset of vertices, and define δ to be the minimum degree of vertices in $\langle U \rangle$. Then

$$\text{comp}(\langle U \rangle) \leq \max\{i: \lambda_i(A) \geq \delta\}.$$

Proof. Let $A = \text{adj}(G)$ and suppose that vertices are numbered so that $U = \{1,\ldots,m\}$. Define z by $z_i = 1$, $i = 1,\ldots,m$; $z_i = 0$, $i = m+1,\ldots,n$. Then (e is a column of 1's)

$$z = \begin{bmatrix} e \\ 0 \end{bmatrix}, \quad A = \begin{bmatrix} B & C \\ C^T & D \end{bmatrix},$$

where $B = \text{adj}(\langle U \rangle)$. Since each entry of Be is the degree of the corresponding vertex, $Be \geq \delta e$. If $B = B_1 \oplus \ldots \oplus B_k$, also $B_k e \geq \delta e$ and then $\lambda_1(B_i) \geq \delta$ for each i. By the lemma, $\lambda_k(A) \geq \delta$, which is equivalent to the conclusion of the theorem. □

Corollary 1. If H is any induced subgraph of a connected graph G, then $\text{comp}(H) \leq \max\{i: \lambda_i(A) \geq 0\}$.

Proof. If B_i is the adjacency matrix of any component of H, then $\lambda_1(B_i) \geq 0$. □

This corollary is similar to a theorem of Cvetković (1971) in which U is chosen to be a maximum set of independent vertices, so that $\text{adj}(U) = 0$. (See Cvetković, et al. (1980) pp. 88-89.)

3. Partitions Determined by Eigenvectors

If the vector z in Theorem B' or Theorem 1 is an eigenvector and $\alpha = \lambda_s(A)$ then in place of an inequality we have the equality $Az = \alpha z$, which holds also if z is replaced by $-z$. Thus the conclusions are strengthened to say that $\langle P \cup 0 \rangle$ and $\langle N \cup 0 \rangle$ have at most $s-1$ components in the case of Theorem B', and that $\langle P \rangle$ and $\langle N \rangle$ have at most $s+m-1$ components in the case of Theorem 1. Here $s = \min\{i: \lambda_i(A) = \alpha\}$ and $m = \text{mult}(\alpha: A)$. For an eigenvector, much more can be learned about the null vertices.

Theorem 3. Let G be connected, $A = \mathrm{adj}(G)$, $Az = \alpha z$ $s = \min\{ i: \lambda_i(A) = \alpha \}$, $m = \mathrm{mult}(\alpha:A)$. Suppose that $\mathcal{O}(z)$ is nonempty and is contained in the set of null vertices for every eigenvector associated with α. Then one of these two cases holds.

(a) No edge joins a vertex of P to one of N, and

$$m + 1 \leq \mathrm{comp}(\langle P \cup N \rangle) \leq s + m - 1.$$

(b) Some edge joins a vertex of P to one of N, and

$$\mathrm{comp}(\langle P \cup N \rangle) \leq s + m - 2.$$

Proof. Let vertices of G be numbered so that

$$z = \begin{bmatrix} x \\ -y \\ 0 \end{bmatrix}, \qquad A = \begin{bmatrix} A_P & A_{PN} & A_{P0} \\ A_{NP} & A_N & A_{N0} \\ A_{0P} & A_{0N} & A_0 \end{bmatrix}, \tag{3}$$

where $A_P = \mathrm{adj}(\langle P \rangle)$ etc. Then the partitioned form of $Az = \alpha z$ yields

$$\begin{aligned} A_P x - A_{PN} y &= \alpha x, \\ A_N y - A_{NP} x &= \alpha y, \\ A_{0P} x - A_{0N} y &= 0. \end{aligned} \tag{4}$$

(a) The hypothesis is that $A_{NP} = A_{PN}^T = 0$. Suppose that

$$B = \begin{bmatrix} A_P & 0 \\ 0 & A_N \end{bmatrix} = \begin{bmatrix} B_1 & & \\ & \ddots & \\ & & B_k \end{bmatrix}, \quad \begin{bmatrix} x \\ -y \end{bmatrix} = \begin{bmatrix} u_1 \\ \vdots \\ u_k \end{bmatrix}$$

where each B_i is irreducible. Note that each u_i is either positive or negative; thus $B_i u_i = \alpha u_i$ implies that

$$\alpha = \lambda_1(B_i), \quad i = 1, \ldots, k.$$

By the lemma and Theorem B, $\lambda_k(A) \geq \alpha$ and $k \leq s + m - 1$.

Now let $[A_{OP}\ A_{ON}] = [C_1, \ldots, C_k]$. Then every eigenvector of A corresponding to α must have the form

$$z = \begin{bmatrix} u_1 \xi_1 \\ \vdots \\ u_k \xi_k \\ 0 \end{bmatrix}$$

because $B_i u_i \xi_i = \alpha u_i \xi_i$ is necessary, and the eigenvector of B_i corresponding to α is unique up to a scalar multiplier. Furthermore, the ξ's must satisfy

$$C_1 u_1 \xi_1 + \ldots + C_k u_k \xi_k = 0 .$$

No C_i can be 0, and no u_i can have a zero element. Thus we have a system of equations whose coefficient matrix has rank 1 at least. The nullity of this system is $m = \text{mult}(\alpha:A)$, so

$$1 + m \leq k .$$

(b) The hypothesis is that $A_{NP} = A_{PN}^T \neq 0$. Suppose P is a permutation matrix such that

$$B = \begin{bmatrix} A_P & A_{PN} \\ A_{NP} & A_N \end{bmatrix} = P \begin{bmatrix} B_1 & & \\ & \ddots & \\ & & B_k \end{bmatrix} P^T, \quad \begin{bmatrix} x \\ -y \end{bmatrix} = P \begin{bmatrix} u_1 \\ \vdots \\ u_k \end{bmatrix},$$

where each B_i is irreducible, and $B_i u_i = \alpha u_i$. There must be $h \geq 1$ of the B_i, say $B_1, \ldots, B_h$, for which u_i has elements of both signs. Thus,

$$\lambda_1(B_i) > \alpha, \quad i = 1, \ldots, h,$$

and so $\lambda_h(B) > \alpha$.

Let $M = \text{mult}(\alpha:B)$, so that

$$h \leq k \leq M.$$

Since at least h eigenvalues of B exceed α and exactly M eigenvalues of B equal α, we have $\lambda_{h+M}(B) \geq \alpha$, or

$$h + M \leq s + m - 1.$$

Because $2h \leq h + M$, we conclude that

$$h \leq (s + m - 1)/2.$$

and because $k \geq M \geq s + m - 1$ and $l \geq h$

$$k = \text{comp}(\langle P \cup N \rangle) \leq s + m - 2. \quad \square$$

Corollary. If $\alpha < 0$ then case (a) is impossible, and in case (b)

$$\text{comp}(\langle P, N \rangle) \leq \max\{i: \lambda_i(A) \geq 0\}$$

Proof. In case (a), $\lambda_1(B_i) = \alpha$ for all i. This is false if $\alpha < 0$, because B_i is nonnegative. The bound cited comes from Corollary 1 of Theorem 2. $\square$

Theorem 3 is particularly interesting when $s = 2$ ($\alpha = \lambda_2(A)$), for then the bounds in case (a) are equal. The proof of part (b) of the following theorem from Powers (1987) uses techniques that do not appear to generalize.

Theorem C. Under the hypotheses of Theorem 3, with $s = 2$, one of these two cases holds

(a) No edge joins a vertex of P to one of N, and $\text{comp}(\langle P \cup N \rangle) = m + 1$.

(b) Some edge joins a vertex of P to one of N, and $\langle P \cup N \rangle$, $\langle P \rangle$, $\langle N \rangle$ are all connected. $\square$

Examples. In Fig. 1, three graphs are shown that illustrate Theorem 2. The first graph has $\lambda_3 = \lambda_4 = 0$. The vertices are labelled with eigenvector components. To satisfy the hypotheses a, b and a + b must be nonzero. For any of these choices, $\text{comp}\langle P \cup N \rangle = 3$, which is the lower bound of part (a) of the Theorem. The second graph, similarly labelled, also has $\lambda_3 = \lambda_4 = 0$, and again a, b and a + b must be nonzero. In this case, $\text{comp}\langle P \cup N \rangle = 4$, which is the upper bound of part (a). This graph also illustrates Corollary 2 of Theorem B'. The first two eigenvalues are $\lambda_1 \cong 2.45$ and $\lambda_2 \cong 0.80$, so bound 1 of case (b) predicts one component for $\langle P \cup 0 \rangle$.

Case (b) of the Theorem is illustrated by the third graph's eigenvalue $\lambda_3 = 1$, which is simple. There are two components in $\langle P \cup N \rangle$, thus realizing the upper bound $s + m - 2 = 2$. Since $\lambda_1 \cong 2.08$, $\lambda_2 \cong 1.57$, both bounds in Corollary 2 of Theorem B' also predict at most two components for $\langle P \cup 0 \rangle$. These examples came from Powers (1986 a,b).

4. Inequalities for Null Elements, Eigenvalues and Multiplicities

The number of null elements in an eigenvector of an adjacency matrix turns out to fit some surprising bounds. A similar study could be made for any non-negative irreducible symmetric matrix.

Theorem 4. Let $A = adj(G)$, G a connected graph on $n > 2$ vertices, $Az = \alpha z$, $\alpha < \lambda_1(A)$, and $\zeta = |0(z)|$. Then

$$\zeta \leq \begin{cases} n - 2 - 2\alpha, & \alpha > 0 \\ n - 2, & -1 < \alpha \leq 0 \\ n - 2|\alpha| & \alpha \leq -1 \end{cases}$$

Proof. Let h and k be such that $z_h \geq z_i \geq z_k$ for all i. First suppose $\alpha > 0$. Then

$$\alpha z_h = \sum_{j=1}^{n} a_{hj} z_j = \Sigma' a_{hj} z_j + \Sigma'' a_{hj} z_j$$

where the first sum includes indices for which $z_j > 0$ and the second those for which $z_j < 0$. Thus

$$\alpha z_h \leq \Sigma' a_{hj} z_j \leq (\pi - 1) z_h$$

$$\alpha |z_k| \leq \Sigma'' a_{kj} |z_j| \leq (\nu - 1)|z_k|$$

where $\pi = |P(z)|$, $\nu = |N(z)|$. The -1 enters because A has 0's on its diagonal. From these inequalities it follows first that

$\alpha \leq \min(\pi, \nu) - 1$, and then that (5)

$$\alpha \leq \frac{\pi+\nu}{2} - 1 = \frac{n-\zeta}{2} - 1. \quad (6)$$

The conclusion of the theorem for $\alpha > 0$ follows from the latter equation.

Next, if $\alpha < -1$, then

$$|\alpha| z_h \leq \sum'' a_{hj} |z_j| \leq \nu |z_k|$$

$$|\alpha| |z_k| \leq \sum' a_{kj} z_j \leq \pi z_h$$

By multiplying the inequalities we find

$$|\alpha| \leq \sqrt{\nu\pi}, \text{ whence} \quad (7)$$

$$|\alpha| \leq \frac{\nu+\pi}{2} = \frac{n-\zeta}{2}. \quad (8)$$

The conclusion of the theorem for $\alpha \leq -1$ is immediate.

Finally, an eigenvector corresponding to $\alpha < \lambda_1(A)$ is orthogonal to a positive vector and thus must have $\pi \geq 1$, $\nu \geq 1$ or $\zeta \leq n - 2$. □

This theorem yields a number of interesting corollaries on bounds for graph eigenvalues.

Corollary 1. If G is a graph on n vertices, then

$$\lambda_2(G) \leq \begin{cases} \frac{n-3}{2} & \text{if } n \text{ is odd,} \\ \frac{n}{2} - 1 & \text{if } n \text{ is even} \end{cases}$$

The bound is achieved if n is odd and is asymptotically sharp if n is even.

Proof. The bounds follow from Eq. (5). For $n = 2m + 1$, take two copies of the complete graph on m vertices, K_m, and add a vertex n adjacent to one vertex in each of the K_m. The second eigenvalue of this graph is easily found to be $m - 1 = (n-3)/2$. The corresponding eigenvector has $z_n = 0$.

For $n = 2m$, take two copies of K_m and add an edge from a vertex of one K_m to a vertex of the other. The second eigenvalue of the resulting graph is

$$\lambda_2(G) = \tfrac{1}{2}(m-3 + \sqrt{m^2+2m-3})$$

$$= m - 1 - \frac{1}{m+1} . \qquad \square$$

Corollary 2. If G is a graph on n vertices, then

$$\lambda_n(G) \geq \begin{cases} -\frac{\sqrt{n^2-1}}{2} & \text{if } n \text{ odd} \\ -\frac{n}{2} & \text{if } n \text{ even} \end{cases}$$

Both bounds are achieved.

Proof. The bounds follow from Eq. (7). Both are achieved by complete bipartite graphs: $K_{m,m}$ if $n = 2m$; $K_{m,m+1}$ if $n = 2m + 1$. $\square$

Corollary 3. If G is a connected bipartite graph on n vertices, then

$$\lambda_1(G) \leq \begin{cases} \frac{\sqrt{n^2-1}}{2} & \text{if } n \text{ is odd} \\ \frac{n}{2} & \text{if } n \text{ is even} \end{cases}$$

Both bounds are achieved.

Proof. In a bipartite graph, $\lambda_1 = -\lambda_n$. The result then follows from Corollary 2. $\square$

Corollary 4. If G is a bipartite graph on n vertices, and if $\nu = [n/4]$, then

$$\lambda_2(G) \leq \begin{cases} \nu & \text{if } n = 4\nu \text{ or } 4\nu + 1 \\ \sqrt{\nu(\nu+1)} & \text{if } n = 4\nu + 2 \text{ or } 4\nu + 3. \end{cases}$$

Proof. Let A be the adjacency matrix of G, z an eigenvector corresponding to $\alpha = \lambda_2(A)$, and suppose that z and A are as in Eq. (3). From Eq. (4) it is easily seen that $\lambda_2(A) \leq \lambda_1(A_P)$ and $\lambda_2(A) \leq \lambda_1(A_N)$. Let H_P be a component

of $\langle P \rangle$ for which $\lambda_1(H_P) = \lambda_1(A_P)$, and analogously $\lambda_1(H_N) = \lambda_1(A_N)$. Then

$$\lambda_2(A) \leq \min\{\lambda_1(H_P), \lambda_1(H_N)\}.$$

The smaller of H_1 and H_2 has at most $[n/2]$ vertices. Now application of Corollary 3 gives the desired result. □

Corollary 5. If α is an eigenvalue of $A = \mathrm{adj}(G)$, where G is a connected graph, then

$$\mathrm{mult}(\alpha:A) \leq \begin{cases} n-2\alpha-1, & 0 < \alpha \\ n-1, & -1 < \alpha \leq 0 \\ n-2|\alpha|+1, & \alpha \leq -1 \end{cases}$$

Proof. If α is an eigenvalue witn multiplicity m, a corresponding eigenvector can be constructed with m - 1 zero entries. The result follows by replacing ζ in Theorem 4 by m - 1. □

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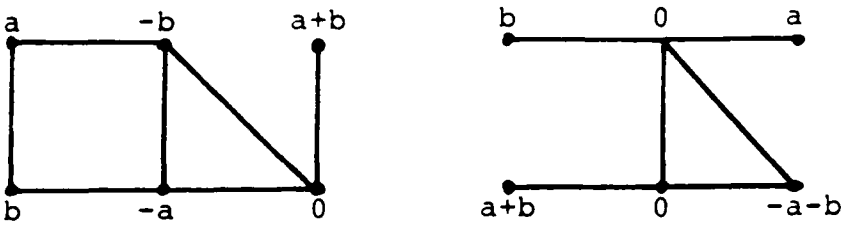

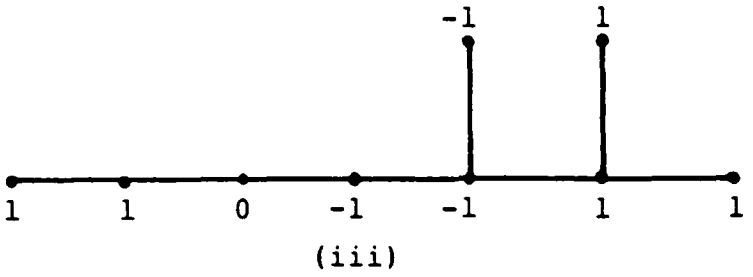

Figure 1 for "Graph Partitioning by eigenvectors" by D.L. Powers
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