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Abstract. Let z be an eigenvector of the adjacency matrix A of a connected graph G. Say a vertix is positive, nonnegative, zero, etc. if the same is true of the corresponding element of z. If z is an eigenvector for the second largest eigenvalue of A, it is known that the nonnegative vertices of G form a connected subgraph. This separation of vertices according to sign provides the basis for studying the structure of G as revealed by its eigenvectors, inequalities on the number of edges joining positive and negative vertices, bounds on the number of zero vertices, bounds on multiplicities and some description of the variability of the elements of z.

The rows of an eigenmatrix provide a mapping of the vertices of G into m-dimensional euclidean space. Some graphs thus "draw themselves". This phenomenon is especially interesting if the graph is the skeleton of a polytope.

Technical Report "Eigenvectors of Graphs"

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1. Structure of a matrix according to an eigenvector.

Let A be a nonnegative symmetric irreducible n x n matrix with eigenvalues $\lambda_1(A) > \lambda_2(A) \geq \ldots \geq \lambda_n(A)$. If z is an eigenvector corresponding to any eigenvalue α other than λ_1, then z has both positive and negative elements. Let rows and columns of A be permuted so that

$$z = \begin{bmatrix} x \\ -y \\ 0 \end{bmatrix} , \qquad A = \begin{bmatrix} A_P & A_{PN} & A_{PO} \\ A_{NP} & A_N & A_{NO} \\ A_{OP} & A_{ON} & A_O \end{bmatrix} \tag{1.1}$$

are partitioned conformally, $x > 0$, $y > 0$.

Fiedler (1975) proved the following.

<u>Theorem</u>. If z is an eigenvector corresponding to eigenvalue $\alpha = \lambda_i(A)$, $i > 1$, then each of the submatrices

$$A_1 = \begin{bmatrix} A_P & A_{PO} \\ A_{OP} & A_O \end{bmatrix} , \qquad A_2 = \begin{bmatrix} A_N & A_{NO} \\ A_{ON} & A_O \end{bmatrix} \tag{1.2}$$

is permutationally similar to a block diagonal matrix having at most $i - 1$ irreducible blocks.

In order to restate this theorem in terms of graphs, define the graph of a nonnegative symmetric n x n matrix A to be gr (A) having vertices $V = \{1 \, . \, . \, n\}$ with i adjacent to j if and only if $a_{ij} > 0$ and $i \neq j$. Then Fiedler's theorem states that each of the graphs gr (A_1), gr (A_2) has at most $i - 1$ connected components. In particular, if $i = 2$ each is a connected graph.

In Eq. (1.1), the last block row and column may be absent (if z has no zero elements). If they are present, then it is enteresting to know their importance to Fiedler's result.

<u>Theorem</u> (Powers 1986) Let $Az = \alpha z$, z and A as in Eq. (1.1), z having some zero elements. Set

$$B = \begin{bmatrix} A_P & A_{PN} \\ A_{NP} & A_N \end{bmatrix} . \tag{1.3}$$

If mult $(\alpha) = \mu > 1$, assume that the elements of z shown equal to 0 in Eq. (1.1) are 0 in every eigenvector of A corresponding to α. If $\alpha = \lambda_2$, exactly one of the following two cases holds.

(1) $A_{PN} = 0$, $\alpha = \lambda_1(A_P) = \lambda_1(A_N)$ and gr (B) has $1 + \mu$ components.

(2) $A_{PN} \neq 0$, $\alpha < \lambda_1(A_P)$, $\lambda_1(A_N)$ and each of the graphs gr (B), gr (A_P), gr (A_N) is connected.

The theorem above can be generalized to the case of eigenvalues after λ_2, as follows:

<u>Theorem</u>. Under the hypotheses of Theorem 1, if $\alpha = \lambda_i < \lambda_{i-1}$, exactly one of the following two cases holds

(1) $A_{PN} = 0$, $\alpha = \lambda_1(A_P) = \lambda_1(A_N)$ and the number k of components in gr (B) satisfies

$$\text{mult}\ (\alpha) + 1 \leq k \leq \text{mult}\ (\alpha) + i - 1.$$

(2) $A_{PN} \neq 0$, $\alpha < \lambda_1(A_P)$, $\lambda_1(A_N)$. The number k of components in gr (B) satisfies

$$k \leq \text{mult}\ (\alpha) + i - 1.$$

2. Cutsize inequalities

The (reordering and) partitioning of a matrix according to the signs of the entries of a given vector, used above, turns out to be a fruitful idea. Suppose G is a connected graph on n vertices, and its vertex set is partitioned into

$$V_1 = \{1, \ldots, m\},\ V_2 = \{m+1, \ldots, m+p\}.$$

Let A, the adjacency matrix of G, be partitioned similarly

$$A = \begin{bmatrix} B & C \\ C' & D \end{bmatrix} \tag{2.1}$$

and define the vectors

$$z = \frac{1}{\sqrt{2}} \begin{bmatrix} e/\sqrt{m} \\ -e/\sqrt{p} \end{bmatrix} \qquad w = \frac{1}{\sqrt{2}} \begin{bmatrix} e/\sqrt{m} \\ e/\sqrt{p} \end{bmatrix}$$

where $e = [1, 1, \ldots, 1]'$. Then $z'z = w'w = 1$, $w'z = 0$. From the extremal properties of $\lambda_1(A)$ and $\lambda_n(A)$ it is easy to show that

$$\lambda_1(A) - \lambda_n(A) \geq \frac{2}{\sqrt{mp}} \; e'Ce. \tag{2.2}$$

But $e'Ce$ is the number of edges of G with one end in V_1 and the other in V_2, i.e., the cutsize for this partition. Thus the difference between largest and smallest eigenvalues of A gives a bound on cutize.

Now suppose that $Az = \alpha z$, α any negative eigenvalue, and

$$z = \begin{bmatrix} x \\ -y \end{bmatrix} \quad , \qquad A = \begin{bmatrix} B & C \\ C' & D \end{bmatrix} \tag{2.3}$$

where $x \geq 0$, $y \geq 0$. Then manipulation of the equation $Az = \alpha z$ in partitioned form leads to the inequality

$$|\alpha|^2 \leq \min\left\{\frac{x'CC'x}{x'x}, \; \frac{y'C'Cy}{y'y}\right\} \quad .$$

Hence one obtains the inequalities

$$|\alpha|^2 \leq \lambda_1(C'C) \leq \mathrm{tr}(C'C) = e'Ce, \tag{2.4}$$

using the fact that $C'C$ is nonnegative definite and C is a matrix of 0's and 1's.

Aspvall and Gilbert (1984) recently proposed using the partition of a graph as given in (2.3), using $\alpha = \lambda_n(A)$, to obtain an approximate 2-coloring. Combining (2.2) and (2.4) we get the bounds

$$\lambda_n^2 \leq e'Ce \leq \frac{\sqrt{mp}}{2}(\lambda_1 - \lambda_n) \tag{2.5}$$

on the cutsize for this partition. These are superior to bounds obtained in the reference cited. Furthermore, the bounds (2.5) are simultaneously achieved if G is the complete bipartic graph $K(m,p)$: $\lambda_1 = -\lambda_n = \sqrt{mp}$.

3. Multiplicities

The investigation in 1 above lead to the question: how many elements of an eigenvector can be 0? If A is the adjacency matrix of a graph on n vertices, and $Az = \alpha z$, let

$$\omega = \#\{\, i:\ z_i = 0 \,\}.$$

Consideration of the rows of the matrix equation $Az = \alpha z$ leads to the inequalities

$$\omega \le n - 2 - 2\alpha, \quad \text{if } 0 \le \alpha \le \lambda_2(A), \tag{3.1}$$

$$\omega \le n - 2|\alpha|, \quad \text{if } \alpha < 0. \tag{3.2}$$

Next, suppose that is an eigenvalue with multiplicity m, and set

$$\Omega = \#\{\, i:\ z_i = 0 \ \text{ if } \ Az = \alpha z \,\}$$

A linear combination of eigenvectors corresponding to α can be forced to have $\omega = m - 1 + \Omega$ zero elements. In combination with (3.1) and (3.2) this fact yields

$$m + \Omega + 2|\alpha| \le \begin{cases} n - 1, & 0 \le \alpha \le \lambda_2(A) \\ n + 1, & \alpha < 0 \end{cases} \tag{3.3}$$

Taking the extreme case $\Omega = 0$ in (3.3) produces the surprising inequality

$$m = \text{mult}\,(\alpha) \le \begin{cases} n - 1 - 2\alpha, & 0 \le \alpha \le \lambda_2(A) \\ n + 1 + 2\alpha, & \alpha < 0 \end{cases} \tag{3.4}$$

Again taking the extreme case $m = 1$ in (3.4) produces two universal bounds

$$\lambda_2(A) \le \frac{n}{2} - 1, \tag{3.5}$$

$$\lambda_n(A) \ge -\frac{n}{2}. \tag{3.6}$$

The second is achieved for $G = K(\frac{n}{2}, \frac{n}{2})$ and the first is approached asymptotically as n increases. Apparently, these inequalities are of some use in the theory of optimal block designs (Jacroux, 1980).

4. Magnitudes of elements in an eigenvector.

For an adjacency matrix A, let $Az = \alpha z$, $0 \leq \alpha \leq \lambda_2(A)$. By considering the rows of the matrix equality $Az = \alpha z$ and separating the positive and negative elements of z, it is easy to prove

$$\frac{\max z_i - \min z_i}{\Sigma |z_i|} \leq \frac{1}{\alpha + 1} \tag{4.1}$$

If $z = \begin{bmatrix} x \\ -y \end{bmatrix}$ with $x \geq 0$, $y \geq 0$, then (4.1) can be restated as

$$\frac{||x||_\infty + ||y||_\infty}{||x||_1 + ||y||_1} \leq \frac{1}{\alpha + 1} \tag{4.2}$$

and in fact it is true that

$$\frac{||x||_\infty}{||x||_1} \leq \frac{1}{\alpha + 1}, \qquad \frac{||y||_\infty}{||y||_1} \leq \frac{1}{\alpha + 1} \tag{4.3}$$

In all these inequalities the left-hand side provides a measure of the variability of the elements of the vector.

By similar means one can establish a double inequality for the variability of the elements of the positive eigenvector z corresponding to $\alpha = \lambda_1(A)$:

$$\frac{\alpha}{2q} \leq \frac{\max z_i}{\Sigma z_i} \leq \frac{1}{\alpha + 1}\,. \tag{4.4}$$

The parameter q on the left is the number of edges in the graph.

Experiments with randomly chosen graphs of orders 10 to 20 indicated that the inequality (4.1) is often an equality.

5. Eigenvector geometry

Let A be the adjacency matrix of a connected graph G on n vertices. Let α be an eigenvalue of multiplicity $m \geq 2$ and Z an n x m matrix of orthonormal eigenvectors. All such Z's can be obtained from any one by forming products ZQ, where Q is an m x m orthogonal matrix.

There is an obvious mapping ϕ from vertices of G to the set $C = \{ e_i^T Z \}$ (where e_i is the ith column of I), interpreted as a set of points in m-dimensional Eüclidean space. If ϕ is 1 to 1, we say that G is m-autographic for α, for the following reason. Draw a line segment between points of C if and only if an edge joins corresponding vertices of G. The result is a structure that realizes G in m-dimensional space. Graphs that are 2- or 3-autographic for some eigenvalue α are particularly interesting, since they "draw themselves" in an easily visualized way.

As a basis for establishing sufficient conditions for the m-autographic property, we have two theorems.

Theorem. (Godsil 1978) Let G be a connected graph, and let the distinct eigenvalues of its adjacency matrix have multiplicities $m_1, \ldots, m_k$. Then the automorphism group of G is contained in the direct sum of the orthogonal groups of degrees $m_1, \ldots, m_k$.

Theorem. (Godsil 1978, Powers 1981). For fixed α and z, let $B_1, \ldots, B_s$ be the preimages under ϕ of the points of C. Then $B_1, \ldots, B_s$ are blocks of the automorphism group of G.

From the first theorem, one can see that if the automorphism group contains say A_4 or S_4, then some eigenvalue has multiplicity 3 or greater. The second theorem shows, e.g., for the graph of the cube that there are 1, 2, 4, or 8 blocks.

If the convex hull of C is a polytope whose skeleton is G , we say that the polytope (and the graph) have the self-reproducing property. We have found many examples including the platonic solids, the 24-cell, and all the regular polytopes of dimension 5 or more. There are also many nonregular polytopes having the self-reproducing property. For example, if we truncate the corners of a cube, or truncate four corners, each across a face diagonal from the others, or erect a pyramid on each face, the resulting polytope has the property. Note that in all these cases, the polytope remains an automorphism group that contains S_4.

We are presently attempting to characterized graphs with the autographic and self-reproducing properties.

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