J. Soc. Indust. Appl. Math.
Vol. 8, No. 2, June, 1960
Printed in U.S.A.

ON THE EIGENVALUES AND EIGENVECTORS OF A CLASS OF MATRICES*[1]

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1. Introduction. Matrices of a particular "structure" frequently appear in various fields of applied mathematics. The matrices considered in this note are generalizations of the matrices which describe "compartment" problems. These occur in such diverse areas as mathematical biophysics (see Hearon [4]) and the study of dielectric relaxation (see Goldberg [2]). Also, some facts about certain special matrices of this kind are used in the Givens method of determining eigenvalues and eigenvectors of symmetric matrices, (see Givens [1]).

With each such matrix A we associate a linear graph $G(A)$. It will then appear that certain properties of the Jordan canonical form of A can be expressed in terms of the topology of $G(A)$. The use of the associated graph is not entirely new, having already appeared in the work of D. Rosenblatt [7] and K. Symanzik [8] and F. Harary.

In §2 we develop the relationship between matrix and graph. In particular, we will give a graph-theoretic interpretation to some of the conditions of Hearon and Goldberg.[2] At this point we restrict ourselves to the special case where $G(A)$ is a sign-symmetric "tree." In this case the work of Hearon and Goldberg [4, 2, 3] implies that A is similar to a real symmetric matrix. We then state our major result on the occurrence of multiple eigenvalues: A necessary and sufficient condition that λ be a multiple eigenvalue of A is that there should exist a point $p \in G(A)$ of order $\geqq 3$ such that λ is an eigenvalue of at least 3 of the branches joined to p. In §3 we prove this result, in §4 we apply it to some simple cases, and in §5 some examples are described which illustrate the importance of the "tree" condition.

2. Formulation of the problem. Consider a real square matrix $A = (a_{ij})$ of order n. With each index i we associate a "point" p_i. If either $a_{ij} \neq 0$ or $a_{ji} \neq 0$ $(i \neq j)$, we associate an "arc" directly connecting p_i and p_j.

* Received by the editors September 3, 1958 and in revised form November 10, 1959.

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[1] This paper was prepared under the auspices of the Atomic Energy Commission at Brookhaven National Laboratory, Upton, L. I.

[2] The author is indebted to the referee for bringing these interesting papers to his attention.

This configuration of "points" and "arcs" is a *graph* $G(A)$. For most of this work we consider *sign-symmetric graphs* where

$$a_{ij} \neq 0 \quad \text{if and only if} \quad a_{ji} \neq 0, \tag{2.1}$$

$$a_{ij}a_{ji} = A_{ij} \geqq 0. \tag{2.2}$$

It is quite natural to consider A_{ij} as being associated with the arc joining p_i to p_j and a_{ij} as being associated with the oriented arc from p_i to p_j.

The theory of graphs has been studied extensively (see [5]). However, for completeness we mention some of the basic concepts.

The graph $G(A)$ is said to be connected if for every two distinct points p and q of $G(A)$ there is a finite sequence of points, say p_k, $k = 1, 2, \cdots, r$ with

$$p = p_1, \qquad q = p_r,$$

and p_i is directly connected to p_{i+1}. With each such path P from p to q we may consider the associated product

$$\pi(P) = a_{12}a_{23} \cdots a_{r-1,r}. \tag{2.3}$$

If it happens that $p = q$, the path is called a *cycle*. It is easy to see that if $G(A)$ is not connected, A is a direct sum of smaller matrices. Hence, in the following, we shall always assume that $G(A)$ is connected.

In the theory of graphs the number of independent cycles is called the *Betti-number* β. Much of the topology of $G(A)$ may be described in terms of the cycles. Correspondingly, the cycles are important in the theory of such matrices. Both Hearon and Goldberg consider the condition

$$a_{i_1 i_2}a_{i_2 i_3} \cdots a_{i_k i_1} = a_{i_1 i_k}a_{i_k i_{k-1}} \cdots a_{i_2 i_1} \tag{2.4}$$

for all $k \leqq n$ and $i_j = 1, 2, \cdots, n$. Hearon showed that if (2.1), (2.2) and (2.4) hold, A is similar to a real symmetric matrix. Goldberg showed that under condition (2.2) and (2.4), A has real eigenvalues. If we consider P^{-1} to mean the path P with the reverse orientation, we can write (2.4) as

$$\pi(P) = \pi(P^{-1}). \tag{2.4a}$$

Neither Hearon nor Goldberg mentioned the concept of a graph. However, Hearon, naturally enough, called a product of the form (2.3) an *r-cycle*, and actually associated it with the corresponding cycle. In order to illustrate that this associated graph is a natural concept in the study of these matrices, we sketch a proof of the following elementary theorem.

THEOREM. *Under conditions* (2.1) *and* (2.2) *the number of* (*algebraically*) *independent relations of the form* (2.4) *is precisely the Betti-number* β *of* $G(A)$.

Proof. If $P_1, P_2, \cdots, P_k$ are independent cycles and P_0 is a given linear combination of them, the relationship (2.4) [or (2.4a)] for P_0 follows from those for $P_1, P_2, \cdots, P_k$. This follows immediately if one associates a "sum" of cycles with a product of associated products, and cancels common terms. Therefore, if N is the number of independent relationships of the form (2.4), $N \leqq \beta$. On the other hand, if $N < \beta$, consider the β_1 independent cycles among the N mentioned in these relationships. Then $\beta_1 = N < \beta$ because the above remark shows that all N relationships follow from the β_1 relationships. Hence these β_1 products, or cycles, determine all the relationships of the form (2.4). However, these β_1 cycles determine a smaller graph G_1, that is, there are arcs in G which do not appear in G_1. In other words, there are $a_{ij} \neq 0$ which do not appear among the original β_1 relationships. However, these terms do appear in some of the relationships required for G. Therefore all such relationships cannot be obtained from the β_1 relationships.

DEFINITION 1. The graph $G(A)$ is called a *tree*, if

(a) $G(A)$ is connected, and
(b) the Betti-number $\beta = 0$.

In all of the following, except for specific examples, we shall assume $G(A)$ is a tree.

THEOREM A. *Under conditions* (2.1) *and* (2.2), *if* $G(A)$ *is a tree*, A *is similar to a real symmetric matrix. Hence* A *can be diagonalized and has real eigenvalues.*

Proof. This is one of Hearon's results which can be seen to follow from the previous theorem and his general theorem.

If $G(A)$ is a tree, then there is a unique path from p to q which involves a minimum number of distinct arcs. We call that number the *distance* from p to q, $d(p, q)$. For example, if $A_{ij} \neq 0$, $d(p_i, p_j) = 1$.

DEFINITION 2. *A point* p *is of order* k *if there are exactly* k *distinct points* q *satisfying*

$$d(p, q) = 1.$$

A few notational remarks are needed.

N1. Points will be denoted by lower case letters, usually p, q, r.

N2. To avoid (as much as possible) the use of subscripts, we will sometimes use the following notation: If p_i is called p and p_j is called q, then a_{ij} will sometimes be designated by a_{pq}, and A_{ij} by A_{pq}.

N3. We imagine the matrix A to be fixed, and refer to $G(A)$ as G.

N4. $B(p, q, G)$ will denote that connected subtree (or *branch*) of the graph G, containing the point p, obtained by removing the arc connecting p to q.

N5. $G(\lambda)$ will denote the characteristic polynomial of the tree G, i.e., of the matrix A. Similarly, $B(p, q, G: \lambda)$ will denote the characteristic polynomial of the subtree $B(p, q, G)$.

THEOREM B. *Under conditions* (2.1) *and* (2.2), *a necessary and sufficient condition that a value λ be a multiple eigenvalue of A is that there exist a point p of order $\geqq 3$ such that λ is an eigenvalue of at least three of the branches at p. That is, for at least three points, say p_1, p_2, p_3, with*

$$d(p_i, p) = 1 \qquad (i = 1, 2, 3)$$

we have

$$B(p_i, p, G: \lambda) = 0.$$

3. Proof of Theorem B. Let $G(\lambda)$ be the characteristic equation of the tree G. Define

$$g_i(\lambda) = a_{ii} - \lambda,$$

and consider $G(\lambda)$ as a function of the $g_i(\lambda)$. We observe that the determinant obtained from $G(\lambda)$ by deleting the ith row and column is also

$$\frac{\partial}{\partial g_i} G(\lambda).$$

N6. If $G(\lambda)$ is the characteristic determinant associated with the tree G, we define $\partial G/\partial p$ to be $\partial G/\partial g_i$ where $p = p_i$. We remark, if G consists of only the point p, i.e., $G(\lambda) = g_p(\lambda)$, then

$$\frac{\partial}{\partial p} G(\lambda) = 1.$$

From the above comments we observe that the operator $\partial/\partial p$ is a partial derivative operator. In particular, the rules for operating on sums and products are valid.

It is particularly useful to have a special notation for the derivative (with respect to p) of the polynomial $B(p, q, G: \lambda)$.

N7. $$\frac{\partial}{\partial p} B(p, q, G: \lambda) = B'(p, q, G: \lambda).$$

We remark

N8. $$\frac{\partial}{\partial q} B(p, q, G: \lambda) = 0.$$

Our first aim is to obtain two formulae for $G(\lambda)$ which reflect our interest in the tree structure. Both of these formulae may be obtained as special cases of the classical identity[3]

$$\det \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \det A_{11} \det (A_{22} - A_{21} A_{11}^{-1} A_{12}).$$

However, it is also easy to get these formulae directly from the form of the determinant.

If we first focus our attention on a particular arc connecting p and q, $G(\lambda)$ is of the form

$$\begin{vmatrix} \boxed{B(p, q, G\colon \lambda)} & a_{pq} \\ a_{qp} & \boxed{B(q, p, G\colon \lambda)} \end{vmatrix} . \tag{3.1}$$

LEMMA 1.

$$G(\lambda) = B(p, q, G\colon\lambda)B(q, p, G\colon\lambda) - A_{pq}B'(p, q, G\colon\lambda)B'(q, p, G\colon\lambda). \tag{3.1a}$$

On the other hand, if we focus our attention on a particular point, say q, and all of the branches at q, we find the form

$$\begin{vmatrix} g_q & a_{q1} & a_{q2} & \cdots & a_{qk} \\ a_{1q} & \boxed{B(1, q, G\colon \lambda)} & & & \\ a_{2q} & & \boxed{B(2, q, G\colon \lambda)} & & \\ \vdots & & & \ddots & \\ a_{kq} & & & & \boxed{B(k, q, G\colon \lambda)} \end{vmatrix} , \tag{3.2}$$

where we have written $1, 2, \cdots, k$ instead of $p_1, p_2, \cdots, p_k$.

LEMMA 2.

$$G(\lambda) = g_q(\lambda) \prod_p B(p, q, G\colon\lambda) - \sum_p A_{pq}B'(p, q, G\colon \lambda) \prod_{p' \neq p} B(p', q, G\colon \lambda) \tag{3.2a}$$

[3] The author is again indebted to the referee for pointing out that these formulae are special cases of this identity.

LEMMA 3.

$$\frac{\partial}{\partial p} G(\lambda) = B'(p, q, G: \lambda) B(q, p, G: \lambda) \tag{3.3a}$$

where q is any point such that $d(p, q) = 1$.

$$\frac{\partial}{\partial p} G(\lambda) = \prod_q B(q, p, G: \lambda) \tag{3.3b}$$

where q runs over all values such that $d(p, q) = 1$.

Proof. Direct computation using formulae (3.1a) and (3.2a).

For the remainder of this section, we restrict ourselves to sign-symmetric trees, i.e., to matrices satisfying (2.1) and (2.2) whose associated graph is a tree.

We proceed with the proof of Theorem B. The "if" part follows directly from (3.2a). Namely, if the characteristic polynomials of at least 3 branches at q vanish for a certain value of λ, each term of (3.2a) has at least a double root.

We now show how the eigenvectors of A are obtained in terms of the vectors of the three branches at q. There is no loss in assuming that points 1, 2, and 3 are the neighbors of q whose branches have λ as an eigenvalue. We refer now to the form (3.2). Let $X = (x_1, x_2, \cdots, x_r)$, $Y = (y_1, y_2, \cdots, y_s)$ and $Z = (z_1, z_2, \cdots, z_m)$ respectively be eigenvectors of $B(1, q, G)$, $B(2, q, G)$ and $B(3, q, G)$ associated with the eigenvalue λ. We may also assume that x_1, y_1, z_1 are the variables associated with the points 1, 2 and 3.

Case 1. $x_1 \neq 0$, $y_1 \neq 0$, $z_1 \neq 0$.

Pick a and b such that

$$a a_{q1} x_1 + b a_{q2} y_1 = 0.$$

Then the vector $aX \oplus bY$ is an eigenvector; i.e., the vector (ξ_i) where

$$\xi_i = \begin{cases} a x_i & \text{if} \quad p_i \in B(1, q, G), \\ b y_i & \text{if} \quad p_i \in B(2, q, G), \\ 0 & \text{otherwise.} \end{cases}$$

Now pick c and d such that

$$c a_{q1} x_1 + d a_{q3} z_1 = 0.$$

Then the vector $cX \oplus dZ$ is an eigenvector. Thus we have exhibited two linearly independent eigenvectors.

Case 2. $x_1 = 0$.

Then the vector $X \oplus \mathbf{0}$ is an eigenvector, where $\mathbf{0}$ is the zero vector.

Case 2a. $y_1 z_1 \neq 0$.

Pick a and b such that

$$a a_{q2} y_1 + b a_{q3} z_1 = 0.$$

The vector $aY + bZ$ is a second linearly independent eigenvector.

Case 2*b*. Either y_1 or $z_1 = 0$, say y_1. Then the vector $Y \oplus \mathbf{0}$ is a second linearly independent eigenvector.

Hence, after completing the "only if" part of the proof, we will not only have a criterion for multiple eignvalues, but we will also be able to construct the associated eigenvectors from the eigenvectors of smaller matrices.

The proof of the "only if" part of theorem B will depend on some lemmas which connect the simultaneous vanishing of $G(\lambda)$ and $(\partial/\partial p)G(\lambda)$, with the order of p in G. Then, the crucial step will involve a procedure of "marching" along the graph G. Because G is a tree, at every point it is possible to choose to march along an arc which takes us further away from our starting point. As we shall see, this plays an important role in the proof.

LEMMA 4. *Let G consist of points of order* $\leqq 2$. (It is easy to see that G is a chain: p_1-p_2-p_3- $\cdots$ -p_n, with exactly two end-points.) *Let p be an end-point. Let $G(\lambda) = 0$. Then*

$$\frac{\partial}{\partial p} G(\lambda) \neq 0.$$

Proof. This is well known, and can be proved by a modification of Givens' proof that the eigenvalues of a symmetric Jacobi matrix which is not the direct sum of smaller Jacobi-matrices are distinct.

LEMMA 5. *Let p be an end-point of G. Let $G(\lambda) = 0$. Let q be that unique point such that $d(p, q) = 1$. Then*

$$\frac{\partial}{\partial p} G(\lambda) = 0 \quad \textit{implies} \quad \frac{\partial}{\partial q} G(\lambda) = 0.$$

Proof. Consider the arc connecting p to q, apply (3.1a) and the hypothesis.

LEMMA 6. *Let p be a point of order 2. Let $G(\lambda) = 0$. Let q and r be two points such that*

$$d(p, q) = d(p, r) = 1.$$

If

$$\frac{\partial}{\partial p} G(\lambda) = 0,$$

then

$$B(r, p, G\colon \lambda) B(q, p, G\colon \lambda) = 0. \tag{3.4a}$$

Moreover, if in addition we have

$$\frac{\partial}{\partial q} G(\lambda) = 0, \tag{3.4b}$$

then

$$\frac{\partial}{\partial r} G(\lambda) = 0. \tag{3.4c}$$

Proof. (3.4a) is merely the restatement of the hypothesis in terms of (3.3b). The rest follows by direct computation using (3.1a) and (3.2a) for the trees $B(q, p, G)$ and $B(r, p, G)$.

Suppose now that for some value λ and some end-point p we have

$$G(\lambda) = \frac{\partial}{\partial p} G(\lambda) = 0.$$

By Lemma 4, G contains at least one point of order $\geqq 3$. Moreover if the point q is the point of order $\geqq 3$ nearest to p, Lemma 5 together with the repeated use of Lemma 6 gives the following:

$$\frac{\partial}{\partial r} G(\lambda) = 0$$

for all points r such that

$$d(p, r) \leqq d(p, q).$$

In particular,

$$\frac{\partial}{\partial q} G(\lambda) = 0.$$

This argument illustrates the "marching" procedure referred to previously. By Lemma 3, λ is an eigenvalue of at least one branch at q. Suppose this is the branch containing p, the end-point. Let "1" be the point on that branch nearest q. We then have $B(1, q, G\colon \lambda) = 0$. However, by hypothesis, $B(1, q, g)$ is a chain as described in Lemma 4. Therefore $B'(1, q, G\colon \lambda) \neq 0$. Referring now to Lemma 2, we see that some other branch at q must also have λ as an eigenvalue.

Therefore, we have proved that at least one branch at q, not containing the end-point p, has λ as an eigenvalue. Let "2" be the point on that branch nearest q. Thus

$$B(2, q, G\colon \lambda) = 0.$$

If $B'(2, q, G\colon \lambda) = 0$ we can repeat the above argument for the tree $G_1 = B(2, q, G)$. However, since G has only a finite number of points of order

$\geqq 3$, this marching procedure must stop. Notice that since we always used a branch *not* containing the initial end-point, the branch of the last subtree G_r such that

$$B(p', q', G_r : \lambda) = 0$$

and

$$B'(p', q', G_r : \lambda) \neq 0$$

is also a branch of G. Thus we have the following result.

LEMMA 7. *Let G be a tree. Let $G(\lambda) = 0$. Let p be an end-point of G such that*

$$\frac{\partial}{\partial p} G(\lambda) = 0.$$

Then G contains a point of order $\geqq 3$, say q, such that for at least one neighbor of q, say r, we have

$$B(r, q, G: \lambda) = 0, \qquad B'(r, q, G: \lambda) \neq 0.$$

If $G(\lambda)$ has a double root for a particular value of λ, all minor determinants of order $n - 1$ must vanish because A is diagonalizable by Theorem A. In particular, every principal minor determinant of order $n - 1$ must vanish; i.e.

$$\frac{\partial}{\partial p} G(\lambda) = 0 \qquad \text{(for every } p\text{)}.$$

Hence Lemma 7 enables us to find a point q of order $\geqq 3$ and a special neighbor r so that the conclusion of Lemma 7 holds. Since $G(\lambda) = 0$ also, Lemma 2 implies there is another neighbor, say r', such that

$$B(r', q, G: \lambda) = 0.$$

Hence, our marching procedure based on Lemmas 5 and 6 leads us to the following result.

LEMMA 8. *Let λ be a multiple root of $G(\lambda)$. Then there is a point q of order* 3 *such that for at least two neighbors, say* 1 *and* 2, *we have*

$$B(1, q, G: \lambda) = B(2, q, G: \lambda) = 0$$

Moreover, for at least one of these values, say 2,

$$B'(2, q, G: \lambda) \neq 0.$$

We now undertake another marching procedure. If only two of the submatrices associated with the branches at q have λ as an eigenvalue, we will find a subtree G_1 of G whose associated submatrix also has λ as a multiple eigenvalue. Moreover, we will see that if G_1 meets the conditions of Theorem B, so does G. Since G has only a finite number of points of order $\geqq 3$, Lemma 4 implies that some subtree G_N of G does satisfy our conditions; namely three branches of G_N which meet at a common point, have λ as an eigenvalue. Hence G_{N-1}, G_{N-2}, $\cdots$ and finally G itself must meet this condition.

LEMMA 9. *Let λ be a multiple root of $G(\lambda)$. Let q, 1, 2 be the points in Lemma 8. Suppose no other branch at q has λ as an eigenvalue. Then the subtree $G_1 = B(1, q, G)$ has λ as a multiple eigenvalue.*

Proof. Since the point q and the graph G, as well as the value λ, are fixed in this discussion, we will abbreviate $B(p, q, G: \lambda)$ and $B'(p, q, G: \lambda)$ as $B(p)$ and $B'(p)$ respectively. Then (3.2a) reads

$$G(\lambda) = g\prod\nolimits_p B(p) - \mathrm{A}_{1q}B'(1) \prod\nolimits_{p\neq 1} B(p) - A_{2q}B'(2) \prod\nolimits_{p\neq 2} B(p) + S = 0.$$

where S has a double root at λ.
Since $d/d\lambda)G(\lambda) = 0$, and $\prod_p B(p)$ has a double root at λ, we obtain:

$$A_{1q}B'(1) \frac{d}{d\lambda} \{\prod_{p\neq 1} B(p)\} + A_{2q}B'(2) \frac{d}{d\lambda} \{\prod_{p\neq 2} B(p)\} = 0.$$

Or, after cancelling the nonzero factor $\prod_{p\neq 1, p\neq 2} B(p)$

$$A_{1q}B'(1) \frac{d}{d\lambda} B(2) + A_{2q}B'(2) \frac{d}{d\lambda} B(1) = 0. \tag{3.5}$$

On the other hand, focusing attention on the arc connecting 2 to q, the fact that

$$\frac{\partial}{\partial(2)} G(\lambda) = 0,$$

together with Lemma 1, implies that the tree G_0 obtained by removing the branch $B(2)$ also has λ as an eigenvalue. Using (3.2a) and the vanishing of $B(1)$,

$$G_0(\lambda) = -A_{1q}B'(1)\prod\nolimits_{p'\neq 1, p'\neq 2} B(p') = 0.$$

Therefore

$$B'(1) = 0,$$

and from (3.5)

$$\frac{d}{d\lambda} B(1) = 0.$$

Suppose now that $G_1 = B(1, q, G)$ has a point, say p, of order $\geqq 3$ and at least three of the branches at p have λ as an eigenvalue.

Case 1. The point 1 is *not* on one of these branches. In this case, each of these branches is also a branch of G, therefore G has a point p, of order $\geqq 3$, and at least three of the branches at p have λ as an eigenvalue.

Case 2. The point 1 is on one of these branches, say B_0. However, it is on only one. Therefore, the other two branches of G_1 are also branches of G. Consider the branch of G which consists of this special branch B_0 of G_1, the point q, the branch $B(2, q, G)$ of G, and all other branches $B(p, q, G)$, $p \neq 1$. Call this branch G_2. Upon focusing our attention on the point q Lemma 2 implies that $G_2(\lambda) = 0$.

Thus, the proof of Theorem B is complete.

4. Application. In an important paper on tracer experiments Sheppard and Householder [5] considered the case of n points $p_1, p_2, \cdots, p_n$ each connected to the single point p. They showed: *If the $a_{p_ip_i}$ are all distinct, then all the eigenvalues are distinct.* It is easy to see how this follows from Theorem B.

Consider now two sets of points, say $p_1, p_2, \cdots, p_n$ each connected to a single point p, and $q_1, q_2, \cdots, q_m$ each connected to a single point q, with p connected to q. From Theorem B we see:

If the sets of numbers $a_{p_ip_i}$ and $a_{q_iq_i}$ are separately distinct, i.e.,

$$a_{p_ip_i} = a_{p_kp_k}$$

if and only if

$$p_i = p_k,$$

and

$$a_{q_iq_i} = a_{q_kq_k}$$

if and only if

$$q_i = q_k,$$

the eigenvalues of the tree G are distinct.

5. Examples. In this section we give two examples of matrices satisfying (2.1) and (2.2) whose associated graph is a closed loop. In the first case we find complex eigenvalues while in the second case we find a multiple eigenvalue and only one associated eigenvector.

EXAMPLE 1. For any two real numbers d and e consider the matrix

$$\begin{pmatrix} -1 & d & 0 & e \\ e & -1 & d & 0 \\ 0 & e & -1 & d \\ d & 0 & e & -1 \end{pmatrix} = A.$$

The eigenvalues of A are

$$\lambda_1 = -1 + d + e$$

$$\lambda_2 = -1 - (d + e)$$

$$\lambda_3 = -1 + i(d - e)$$

$$\lambda_4 = -1 - i(d - e).$$

(This example was given by J. Moser).

EXAMPLE 2. For any real number α, consider the matrix

$$\begin{pmatrix} -1 & a & 0 & e \\ a & -1 & \alpha a & 0 \\ 0 & \alpha a & -1 & d \\ d/\alpha & 0 & d & -1 \end{pmatrix} = A.$$

One can verify by direct computation that $\lambda = -1$ is a multiple eigenvalue of A. In fact, in the language of §3, for every p

$$\det (A + I) = \frac{\partial}{\partial p} G(-1) = 0.$$

Moreover, it can be verified that unless

$$e = \frac{d}{\alpha}$$

there is only one associated eigenvector.[4]

In both of these examples, the associated graph consists of four points connected in a loop, i.e.

$$\begin{array}{ccc} p_1 & - & p_2 \\ | & & | \\ p_4 & - & p_3 . \end{array}$$

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[4] There is, of course, a second, independent vector V such that $(A + I)^2V = \mathbf{0}$.

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