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On the Eigenvalues and Eigenvectors of Certain Finite, Vertex-Weighted, Bipartite Graphs

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The established, spectral characterisation of bipartite graphs with unweighted vertices (which are here termed *homogeneous* graphs) is extended to those bipartite graphs (called *heterogeneous*) in which all of the vertices in one set are weighted h_1, and each of those in the other set of the bigraph is weighted h_2. All the eigenvalues of a homogeneous bipartite graph occur in pairs, around zero, while some of the eigenvalues of an arbitrary, heterogeneous graph are paired around $\frac{1}{2}(h_1 + h_2)$, the remainder having the value h_2 (or h_1). The well-documented, explicit relations between the eigenvectors belonging to "paired" eigenvalues of homogeneous graphs are extended to relate the components of the eigenvectors associated with each couple of "paired" eigenvalues of the corresponding heterogeneous graph. Details are also given of the relationships between the eigenvectors of an arbitrary, homogeneous, bipartite graph and those of its heterogeneous analogue.

1. INTRODUCTION

Consider a finite, bipartite graph, G, with vertex set $V = V_1 \cup V_2$, (V_1 and V_2 disjoint) and edge family, E, the elements $(v_i v_j)$ of which are such that exactly one vertex is drawn from each of V_1 and V_2. The number of vertices, $|V|$, in G is N. The number in V_1 will be denoted $|V_1| = m$, and, similarly, $|V_2| = m + p$. (Hence, $N = 2m + p$). Let the weighting, $\rho(V_1)$, of each vertex in V_1 be h_1, and of each vertex in V_2 be $\rho(V_2) = h_2$. Then we shall call such a graph *homogeneous* if $h_1 = h_2$ (both of which can then conveniently, but arbitrarily, be put equal to zero). If $h_1 \neq h_2$, the graph will be

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termed *heterogeneous*. Further, let the ordered family of eigenvalues of the adjacency matrix, $\mathbb{A}(G)$, of G be

$$\Lambda(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_N\} \text{ with } \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_N$$

In 1940, Coulson and Rushbrooke [1] showed that for a homogeneous, bipartite graph in which $h_1 = h_2$ are set equal to zero,

$$\lambda_i + \lambda_{N-i+1} = 0 \tag{1}$$

for all i, $1 \leqslant i \leqslant N$. This characterisation of homogeneous, bipartite graphs is a simple consequence of the Perron-Frobenius theorem on non-negative matrices, and was first proved in the chemical literature, where it is known as the Coulson-Rushbrooke "Pairing" theorem. Since then, however, there have been many graph-theoretical discussions and proofs of it (some of which are independent), both in the mathematical and chemical literature (for references, see [2]). Coulson and Rushbrooke further established a simple relation between the eigenvectors belonging to these "paired" eigenvalues. If $\alpha = (r_1, r_2, \ldots, r_m, s_1, s_2, \ldots, s_{m+p})^T$ is the eigenvector associated with the eigenvalue λ_i, then α^p, the eigenvector giving rise to the paired eigenvalue, λ_{N-i+1}, is

$$\alpha^P = (r_1, r_2, \ldots, r_m, -s_1, -s_2, \ldots, -s_{m+p})^T. \tag{2}$$

One consequence of equation (1) is that, if N is odd, there is an i such that

$$\lambda_i = \lambda_{N-i+1} = 0; \quad \text{clearly,} \quad i = \frac{N+1}{2}.$$

Schwenk, Trinajstić and one of the present authors [2] have recently established an analogous pairing-relation for a restricted class of heterogeneous, bipartite graphs. They required that:

(i) $|V_1| = |V_2|$,

(ii) $\rho(V_1) = h$,

(iii) $\rho(V_2) = 0$.

Then,

$$\lambda_i' + \lambda_{N-i+1}' = h. \tag{3}$$

(λ' denotes an eigenvalue of a heterogeneous graph, whereas λ—unprimed—denotes an eigenvalue of a homogeneous graph.) However, these authors did not find any relation between the eigenvectors associated with each pair of eigenvalues disposed about h (equation (3)); in particular, no eigenvector-relation was found, analogous to the one pointed out by Coulson and Rushbrooke for homogeneous, bipartite graphs.

The object of the present paper, therefore, is to show that an eigenvalue "pairing" arises for any finite, heterogeneous, bipartite graph, to establish its form, and to indicate the relation which exists between the eigenvectors belonging to each couple of paired eigenvalues. In doing this in a graph-theoretical context, we draw freely and rely considerably on the arguments of Bochvar, Stankevich and Chistyakov, [3-5] who encountered and solved what is essentially the same problem (albeit in somewhat disguised form) during their chemical studies of what they termed "truly alternant hetero-conjugated molecules".

2. Pairing of Eigenvalues and Other Eigenvalue Relations

Consider a finite, heterogeneous, bipartite graph G with vertex set $V = V_1 \cup V_2$, $|V_1| = m$, $|V_2| = m + p$, $\rho(V_1) = h_1$, $\rho(V_2) = h_2$. If G is appropriately labelled, its adjacency matrix, $\mathbb{A}(G)$, can be partitioned as follows [3]:

$$\mathbb{A}(G) = \left(\begin{array}{c|c} h_1\mathbb{1}_1 & \mathbb{B} \\ \hline \mathbb{B}^T & h_2\mathbb{1}_2 \end{array}\right)$$
$$\begin{aligned} \dim(\mathbb{1}_1) &= m \times m \\ \dim(\mathbb{1}_2) &= (m+p) \times (m+p) \\ \dim(\mathbb{B}) &= m \times (m+p). \end{aligned} \tag{4}$$

The characteristic equation of G is thus:

$$\left|\begin{array}{c|c} (h_1 - \lambda')\mathbb{1}_1 & \mathbb{B} \\ \hline \mathbb{B}^T & (h_2 - \lambda')\mathbb{1}_2 \end{array}\right| = 0. \tag{5}$$

Bochvar, Stankevich and Chistyakov [3, 4] have shown that the determinant in equation (5) can be written

$$(Y')^p \sum_{i=0}^{m} b_i(-Z')^i = 0,$$

where:

$$\begin{aligned} Y' &= h_2 - \lambda', (X' = h_1 - \lambda'), \\ Z' &= X'Y', \\ & b_i \geqslant 0,\ b_m = 1. \end{aligned} \tag{6}$$

Furthermore,

$$\sum_{i=0}^{m} b_i(-Z')^i = 0 \text{ has } m \text{ solutions}$$

$$Z' \geqslant 0. \text{ Of the } (2m + p) \text{ eigenvalues of } \mathbb{A}(G),$$

p are thus $\lambda' = h_2$, and the remaining $2m$ can be found from

$$(h_1 - \lambda')(h_2 - \lambda') = Z'$$

in which Z' is a solution of (6)

$$\Rightarrow \lambda' = \frac{h_1 + h_2 \pm \{(h_2 - h_1)^2 + 4Z'\}^{1/2}}{2}. \tag{7}$$

We now observe that equation (6) has formally the same roots, $\{Z'\}$, in the heterogeneous case as the $\{Z\}$ which are its roots in the corresponding homogeneous case (for the polynomial represented by the summation-sign in equation (6) has the same coefficients, b_i, in both cases provided that the edge-weightings of G are held constant during transformation to the heterogeneous graph). However, whereas, for the heterogeneous graph, $Z' = (h_1 - \lambda')(h_2 - \lambda')$, in the homogeneous case, $h_1 = h_2 = 0$, the eigenvalues are denoted by λ, and hence, $Z = \lambda^2$. The appropriate values for the $\{Z'\}$, therefore, in equation (7), are $\{\lambda^2\}$, where $|\lambda|$ is the modulus of a couple of paired eigenvalues of the parent homogeneous graph that map onto the two values of λ' given by equation (7) on transformation to the heterogeneous case. We may therefore write (7):

$$\lambda' = \frac{h_1 + h_2 \pm \{(h_2 - h_1)^2 + 4\lambda^2\}^{1/2}}{2}. \tag{8}$$

The spectrum of this general, finite, heterogeneous, bipartite graph is, therefore, as follows:

① p eigenvalues lie at $\lambda' = h_2$; (*i.e.*, there are as many eigenvalues equal to the weighting of the vertices V_2 as there are excess of vertices in V_2 over the number in V_1).

② The remaining $2m$ eigenvalues are paired about the arithmetic mean of the vertex weightings, $(h_1 + h_2)/2$, lying $\frac{1}{2}(\{(h_2 - h_1)^2 + 4\lambda^2\}^{1/2})$ above and below this mean, (where $|\lambda|$ is the modulus of a couple of paired eigenvalues of the corresponding homogeneous bipartite graph which are mapped onto the pair of λ' values given by equation (8), on transformation to the heterogeneous case).

It is readily seen that equation (1) (the Coulson-Rushbrooke theorem) is a special case of the above which occurs when $h_1 = h_2 = 0$, and equation (3) is the special case which arises when $h_1 = h$ (non-zero, in general), $h_2 = 0$ and $p = 0$.

We have already drawn attention to the fact that in the case of a *homo*geneous, bipartite graph ($h_1 = h_2 = 0$) for which N is odd there must arise at least one zero-eigenvalue; this can be rationalised in terms of ①, above, for, if N is odd, there must be an excess of *at least one* in the number of vertices in one vertex subset of the bigraph over the number in the other subset. It will now be appreciated, however, from the general spectrum outlined above, that an arbitrary, *homo*geneous, bipartite graph (where $h_2\,(=h_1) = 0$) in which there is an excess of p vertices in one vertex subset over the number in the other, will have *at least p* zero-eigenvalues. Such zero-eigenvalues of a homogeneous, bipartite graph that are predictable by inspection in this way we shall call *predictable* zero-eigenvalues. In certain instances, however, zero-eigenvalues may arise more capriciously in homogeneous, bipartite graphs, even when such graphs have the same number of vertices in each set ($|V_1| = |V_2|$, ($p = 0$)); (the well-known spectra of the cyclic graphs, C_N, N an integral multiple of 4, are a case in point [6]). Following Longuet-Higgins [7] (who encountered them in a chemical context) we shall call zero-eigenvalues that do not owe their origin to unequal numbers of vertices in the two sets *supernumerary* zero-eigenvalues; from equation (1), it is evident that such supernumerary zeros, when they do arise, must occur in pairs [8].

We may summarise this discussion by using the general spectrum outlined above to consider the eigenvalue mappings that occur on transformation from an arbitrary, homogeneous, bipartite graph (with $|V_2| - |V_1| = p$) to the corresponding heterogeneous one:

(a) The *p predictable* zero-eigenvalues in the homogeneous case will map onto p similarly *predictable* eigenvalues at $\lambda' = h_2$ in the heterogeneous case.

(b) Each pair of non-zero eigenvalues of the homogeneous bipartite graph will map onto two distinct eigenvalues in the heterogeneous case, neither of which is itself h_1 or h_2, but which are paired around the arithmetic mean of h_1 and h_2.

(c) Any pairs of *supernumerary* zeros that are present will map onto two distinct eigenvalues of the heterogeneous graph, one lying at $\lambda' = h_1$ and the other at $\lambda' = h_2$. (This is seen by considering the two roots obtained on substituting $|\lambda| = 0$ into equation (8)). This therefore confirms that, in one important respect, a pair of supernumerary zeros in the homogeneous case behaves no differently from any pair of non-zero eigenvalues in that they both map, on transformation to the heterogeneous case, onto a pair of distinct eigenvalues equally disposed about the mean of h_1 and h_2. By analogy with our previous terminology, any eigenvalues $\lambda' = h_2$ that arise in this way (as opposed to those which are *predictable*) may appropriately be termed "*supernumerary* h_2-eigenvalues".

3. Eigenvector Relations

From Section 2 it is clear that all eigenvectors of a homogeneous, bipartite graph (hereafter called "homo-eigenvectors") that belong to *predictable* zero-eigenvalues are simultaneously hetero-eigenvectors with the associated eigenvalue h_2. The remaining eigenvalues and eigenvectors are paired. Each pair satisfies the relation noted by Coulson and Rushbrooke [1], namely that

$$\begin{pmatrix} \mathbb{O}_1 & \mathbb{B} \\ \mathbb{B}^T & \mathbb{O}_2 \end{pmatrix} \begin{pmatrix} \mathbf{r} \\ \mathbf{s} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{r} \\ \mathbf{s} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathbb{O}_1 & \mathbb{B} \\ \mathbb{B}^T & \mathbb{O}_2 \end{pmatrix} \begin{pmatrix} \mathbf{r} \\ -\mathbf{s} \end{pmatrix} = -\lambda \begin{pmatrix} \mathbf{r} \\ -\mathbf{s} \end{pmatrix}, \tag{9}$$

(in which we have denoted the $(2m + p)$-component vector $\alpha = (r_1, r_2, \ldots, r_m, s_1, s_2, \ldots, s_{m+p})^T$ by $(\mathbf{r}, \mathbf{s})^T$, with:

$$\dim(\mathbf{r}) = m$$
$$\dim(\mathbf{s}) = m + p).$$

We now form the plausible hypothesis that the pair of corresponding eigenvectors in the heterogeneous graph also lies in the two-dimensional subspace generated by $\mathbf{r}$ and $\mathbf{s}$. The eigenvalue equation then takes the form:

$$\begin{pmatrix} h_1\mathbb{1}_1 & \mathbb{B} \\ \mathbb{B}^T & h_2\mathbb{1}_2 \end{pmatrix} \begin{pmatrix} a\,\mathbf{r} \\ b\,\mathbf{s} \end{pmatrix} = \begin{pmatrix} (h_1 a + \lambda b)\,\mathbf{r} \\ (\lambda a + h_2 b)\,\mathbf{s} \end{pmatrix} = \lambda' \begin{pmatrix} a\,\mathbf{r} \\ b\,\mathbf{s} \end{pmatrix}. \tag{10}$$

If $\mathbf{r}$ and $\mathbf{s}$ are individually normalised, we may normalise our presumed eigenvector by setting $a^2 + b^2 = 1$. Thus, we need to solve the system:

$$\begin{aligned} a^2 + b^2 &= 1 \\ \lambda' a &= h_1 a + \lambda b \\ \lambda' b &= \lambda a + h_2 b \end{aligned} \tag{11}$$

for a, b, and the new eigenvalue, λ'. Now whenever $\lambda = 0$ (resulting from a pair of supernumerary zeros in the homogeneous graph), two independent solutions are given by: $a = 1$, $b = 0$, $\lambda' = h_1$ (eigenvector $\mathbf{r}$) and $a = 0$, $b = 1$, $\lambda' = h_2$ (eigenvector $\mathbf{s}$). Otherwise λ may be taken as positive. This gives two solutions with λ' having either value given in (8), a and b then satisfying

$$a^2 = \frac{\lambda' - h_2}{2\lambda' - h_1 - h_2} \quad (>0) \qquad \text{and} \qquad b^2 = \frac{\lambda' - h_1}{2\lambda' - h_1 - h_2} \quad (>0).$$

The sign of a may be taken to be positive while the sign of b will match the sign of $\lambda' - h_1$.

In this way, each pair of non-predictable eigenvalues and their two eigenvectors have been used to generate a two-dimensional subspace in which we were able to identify a pair of hetero-eigenvectors. These, together with the original predictable eigenvectors, form a complete set of eigenvectors for the heterogeneous graph.

4. Concluding Remarks

It should be observed that no step in the present argument has depended on the actual magnitudes of the elements of the sub-matrix $\mathbb{B}$ of the adjacency matrix $\mathbb{A}(G)$. The generalised eigenvalue-pairing theorem for finite, heterogeneous, bipartite graphs reported in this paper (Sect. 2), as well as the explicit relations that have been detailed between the corresponding eigenvectors (Sect. 3), therefore apply equally to arbitrarily edge-weighted graphs of this type, in which off-diagonal elements of $\mathbb{A}(G)$ may take any value, and not merely either 0 or 1—provided that such edge-weightings are held constant during the transformation from the homogeneous bipartite graph to its corresponding heterogeneous analogue.

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