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On the Spectral Invariants of Symmetric Matrices with Applications in the Spectral Graph Theory

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Abstract. We first prove a formula which relates the characteristic polynomial of a matrix (or of a weighted graph), and some invariants obtained from its principal submatrices (resp. vertex deleted subgraphs). Consequently, we express the spectral radius of the observed objects in the form of power series. In particular, as is relevant for the spectral graph theory, we reveal the relationship between spectral radius of a simple graph and its combinatorial structure by counting certain walks in any of its vertex deleted subgraphs. Some computational results are also included in the paper.

1. Introduction

As well-known, square matrices can be interpreted as weighted (di)graphs, and vice versa. Therefore, to a given real square matrix $A = (a_{ij})$, we can associate a weighted (di)graph $G = G(A)$ whose vertex set corresponds to rows (or columns) of A, with two vertices v_i and v_j of G joined by an arc whenever $a_{ij} \neq 0$; then a_{ij} is the weight of this arc. Note, if $v_i = v_j$ then a weighted directed or undirected loop, no matter which, arises. Clearly, if A is symmetric then two arcs joining the same pair of (distinct) vertices can be replaced by a single weighted edge whose weight is a_{ij} $(= a_{ji})$. On the other hand, if a weighted (di)graph G is given then A $(= A(G))$ can be uniquely determined. So square matrices and weighted (di)graphs can be identified. This approach is very common in the combinatorial matrix theory, since many important features of matrices can be revealed just from the structure of the so called underlying (di)graph of the associated weighted (di)graph, i.e. (di)graph without arc or edge weights. For more details on these connections, see for example [3]. Throughout the paper we will restrict ourselves only to symmetric matrices, and thus to weighted graphs.

There are many formulas in the literature (see, for example, [6]) for computing or expressing spectral invariants of matrices, or associated weighted graphs, in terms of their combinatorial structure. For example, in the spectral graph theory the Schwenk formulas for computing (by recursion) the characteristic polynomial of a graph are well-known – see [10], or [1] for the weighted counterpart. In some other formulas various invariants stemming, say from eigenspaces, are included, like graph angles (see, for example, [6]).

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Here we will plug in some purely structural graph invariants, or more precisely, we will include into considerations weighted walks between certain vertices in weighted graphs (or corresponding matrices). Needless to add, any matrix invariant (like spectrum or characteristic polynomial) will be considered as a graph invariant and vice-versa. In addition, every concept from the graph theory, not given here, can be found in [5, 6], or also in [2].

The rest of the paper is organized as follows: in Section 2 we give our main results and in Section 3 we consider some applications, especially in the spectral graph theory; in Section 4 we provide some computational results, while Section 5 is left for a conclusion.

2. Main Results

Let A be a real symmetric matrix of order n, and let A_u be its principal submatrix obtained by deleting the u-th row and column. Interchangeably, in the spirit of Section 1, these two matrices can be considered as weighted graphs G and G_u, respectively. Clearly, G_u is a vertex deleted subgraph of $G = (V(G), E(G))$; so $V(G_u) = V(G) \setminus \{u\}$. Next we have

$$(xI - A_u)^{-1} = x^{-1}(I - \frac{1}{x}A_u)^{-1} = \sum_{k=0}^{\infty} \frac{1}{x^{k+1}} A_u^k, \tag{1}$$

where $|x|$ is sufficiently large (or its reciprocal value sufficiently small). Let U be the set of neighbours of u in G. So $U \subseteq V(G_u)$, and let $\mathbf{w}_U \in \mathbb{R}^{n-1}$ be the weight vector for U in which the v-th entry ($v \neq u$) is equal to (u, v) entry of A. Then, from the above we obtain

$$\mathbf{w}_U^t (xI - A_u)^{-1} \mathbf{w}_U = \sum_{k=0}^{\infty} \frac{W_k(U; G_u)}{x^{k+1}}, \tag{2}$$

where

$$W_k(U; G_u) = \mathbf{w}_U^t A_u^k \mathbf{w}_U. \tag{3}$$

Clearly, $W_k(U; G_u)$ is equal to the sum of weights of all "weighted" walks of length k in G_u which start and terminate in the vertices from U. Recall, the weight of some walk is the product of weights of all edges belonging to the walk in question.

Let

$$A_u = \mu_1 P_1 + \mu_2 P_2 + \cdots + \mu_r P_r \tag{4}$$

be the *spectral decomposition* of A_u. Here $\mu_1, \mu_2, \ldots, \mu_r$ are the distinct eigenvalues of A_u (or G_u), and $P_1, P_2, \ldots, P_r$ are the corresponding projection matrices of A_u (resp. of "labeled graph" G_u). Note also that $\mathbf{w}_U^t P_s \mathbf{w}_U = ||P_s \mathbf{w}_U||^2$, since $P_s^T = P_s$ and $P_s^2 = P_s$. Next we easily obtain

$$\mathbf{w}_U^t [\sum_{s=1}^{r} \frac{P_s}{x - \mu_s}] \mathbf{w}_U = \sum_{k=0}^{\infty} \frac{W_k(U; G_u)}{x^{k+1}}, \tag{5}$$

and therefore

$$\sum_{s=1}^{r} \frac{||P_s \mathbf{w}_U||^2}{x - \mu_s} = \sum_{k=0}^{\infty} \frac{W_k(U; G_u)}{x^{k+1}}. \tag{6}$$

Using the generalized form of Rowlinson's formula (given in [11], see also [6, 9] for its original form) we obtain

$$\Phi_G(x) = \Phi_{G_u}(x)[x - a_{uu} - \sum_{s=1}^{r} \frac{||P_s \mathbf{w}_U||^2}{x - \mu_s}],$$

where Φ stands for the characteristic polynomial of a matrix, or equivalently its corresponding weighted graph. So we easily arrive at the following result:

Theorem 2.1. *Let G (= $G(A)$) be the weighted graph associated to a real symmetric matrix A, and let u be a non-isolated vertex of G, while U the set of neighbours of u in G. If $A_u = A(G_u)$, denote by $W_k(U; G_u)$ the sum of all entries of A_u^k whose indices belong to U. Then, provided the series below converges, we have*

$$x - a_{uu} - \frac{\Phi_G(x)}{\Phi_{G_u}(x)} = \sum_{k=0}^{\infty} \frac{W_k(U; G_u)}{x^{k+1}}. \tag{7}$$

At this place the following remark deserves to be mentioned:

Remark 2.2. *First a_{uu} is a weight of the loop at vertex u and $W_0(U; G_u)$ is equal to the sum of squares of weights of the edges incident to u (note, the loop at u is excluded).*

Secondly, in the case that A is a symmetric non-negative matrix, which is also irreducible (then G is connected), the question of convergence of the above series can be resolved as follows. By the spectral decomposition (cf. (4)) we easily obtain

$$W_k(U; G_u) = \mathbf{w}_U^t A_u^k \mathbf{w}_U = \mu_1^k sum(P_1; U) + \mu_2^k sum(P_2; U) + \cdots + \mu_r^k sum(P_r; U), \tag{8}$$

where $sum(P_i; U)$ denotes the sum of all entries of P_i whose both indices belong to U. Actually, $W_k(U; G_u)$ is a sum of weights of all (weighted) walks of length k in G_u which start and terminate in the vertices from U. Next, with our assumptions, for large values of k, $W_k(U; G_u)$ is asymptotically equivalent to $c\mu_1^k$, for some constant c (note μ_1 is the largest eigenvalue of A_u). So, if $|x| > \mu_1$ we indeed have a convergence due to standard tools on power series.

In particular, if $x = \rho$, where ρ is a spectral radius of A (or also of G), then in view of the above remark $\rho > \mu_1$, and the convergence does hold (if necessary, see [5] Subsection 0.3, with focus on non-negative matrices and Interlacing theorem). Therefore we arrive at the following result:

Corollary 2.3. *Let A be be a real symmetric non-negative irreducible matrix, and let $G = G(A)$. Let u be a vertex of G and U the set of neighbours of u, and let $A_u = A(G_u)$. Denote by $W_k(U; G_u)$ the sum of all entries of A_u^k whose indices belong to U (see (3)). Then ρ, the spectral radius of G, satisfies*

$$\rho = a_{uu} + \sum_{k=0}^{\infty} \frac{W_k(U; G_u)}{\rho^{k+1}}. \tag{9}$$

In particular, under the same assumptions, if the underlying graph of G is bipartite then

$$\rho = a_{uu} + \sum_{k=0}^{\infty} \frac{W_{2k}(U; G_u)}{\rho^{2k+1}}. \tag{10}$$

Proof. First, (9) follows from (7) by putting in it $x = \rho$ (see also Remark 2.2). Secondly, if G is bipartite then, clearly, $W_{2k+1} = 0$ for each k and we immediately obtain (10). Alternatively, by putting in (9) that $x = \pm\rho$ and summing up the obtained expressions we also arrive at (10). □

3. Applications in the Spectral Graph Theory

In the spectral graph theory, we usually consider simple graphs, i.e. finite undirected graphs without loops or multiple edges. Then the quantity $W_k(U; G)$ defined in Section 2 (cf. (3)) for a given graph $G = (V, E)$ and its vertex subset $U \subset V$ counts just the walks of length k which start and terminate in the vertices from U. So $W_k(U; G_u)$ has a nice combinatorial interpretation. Further on we will also use the notation

$$\mathcal{W}(U; G) := (W_0(U; G), W_1(U; G), \ldots) \tag{11}$$

to stand for a corresponding walk sequence of G.

We now consider various applications of the results from Section 2 having in view their combinatorial interpretations pointed above. In particular, we will pay attention on the following subtopics:

(i) Generating functions: Let

$$g(x;U) := \sum_{k=0}^{\infty} W_k(U;G)x^k \tag{12}$$

be the generating function for the number of walks of length k in a simple graph G which start and terminate in the vertices belonging to the subset U of $V(G)$. Using Theorem 2.1 (see (7)) we obtain

$$g(x;U) = \frac{1}{x^2} - \frac{1}{x}\frac{\Phi_{G^u}(\frac{1}{x})}{\Phi_G(\frac{1}{x})}, \tag{13}$$

where G^u is a supergraph of G obtained by adding to G a vertex u adjacent only to vertices from U.

In particular, if U is a singleton, say $U = \{v\}$, then by using [5, Formula (2.2)], i.e. the particular case of Schewenk's formula (see (19)), we then obtain

$$g(x;U) = \frac{1}{x}\frac{\Phi_{G_v}(\frac{1}{x})}{\Phi_G(\frac{1}{x})}. \tag{14}$$

Needless to add, then only closed walks which start and terminate in v are counted. On the other hand, if $U = V(G)$, i.e. if it is the whole vertex set of G, then all possible walks in G are counted.

Remark 3.1. *First, the problem of counting walks in graphs is widely studied in the literature, among others due to considerable interest in chemistry and physics (see, for example, [5]). At this place we emphasize the fact that the closed walks of some graph starting and terminating at the fixed vertex are mostly studied (then (14) is used). Note also that all walks in G of length k starting and terminating in U are not in one-to-one correspondence with all closed walks in G^u of length $k+2$ starting and terminating at vertex u in G^u.*

Secondly, for us it is noteworthy that powers of the adjacency matrix can be easily computed either by using recurrent relations based on the minimal polynomial (whose degree is the number of distinct eigenvalues), or by using the spectral decomposition technique.

Thirdly, the following result from [7] deserves to be mentioned here: given a graph $G = (V, E)$ on n vertices then

$$W_k(V;G) \leq d_1^k + d_2^k + \cdots + d_n^k, \tag{15}$$

where $d_1, d_2, \ldots, d_n$ are its (vertex) degrees. Equality holds if and only if G is regular.

(ii) Cospectral vertex deleted subgraphs: Let G be a (simple) graph, while G_v and G_w its vertex deleted subgraphs obtained by deleting vertices v and w, respectively. If v and w have the same degrees (this is always possible in any simple non-trivial graph) then G_v and G_w can be cospectral, i.e. share the same spectrum. Applying Theorem 2.1 we obtain the following a bit more general result:

Theorem 3.2. *Let G_v and H_w be the vertex deleted subgraphs of two cospectral graphs G and H, respectively. Then G_v and H_w are cospectral if and only if*

$$\mathcal{W}(U_v;G_v) = \mathcal{W}(U_w;H_w), \tag{16}$$

where U_v are the neighbours of v in G, while U_w are the neighbours of w in H.

Consider next the well-known Ulam conjecture, and assume that it is false. Let (G, H) be a counter-example pair. Recall, as pointed by Tutte in [12], G and H are cospectral. Then, for each $v \in V(G)$, there exists $w \in V(H)$ such that G_v and H_w are isomorphic. Let U_v and U_w be the neighbours of v in G and of w in H, respectively. Then, by Theorem 3.2, we have that $\mathcal{W}(U_v;G_v) = \mathcal{W}(U_w;H_w)$.

Theorem 3.2 also holds if G and H coincide. Then the problem of cospectrality of G_v and G_w arises. It turns to be important in studying perfect state transfer in graphs (see, for example, [8] for more details). See also the first part of Remark 3.1. Next, following Godsil and his slides from 2011 we have:

Two vertices v and w in the graph G are cospectral, or equivalently G_v and G_w are cospectral if and only if any of the following (equivalent) conditions holds:

(i) $\|P_i \mathbf{e}_v\| = \|P_i \mathbf{e}_w\|$ for each i i.e. the corresponding quantities are the same (see [6, Proposition 2.2.6]);

(ii) the generating function for the closed walks in G starting at v is equal to the generating function for the closed walks in G starting at w;

(iii) the generating function for the walks in G_v starting at vertex in U_v (the neighbourhood of v in G) and terminating also in U_v is equal to the generating function for the walks in G_w starting at U_w (the neighbourhood of w in G) and terminating also in U_w.

Recall, the quantities appearing in item (i) are called graph angles (see, for example, [6]). Note also that in item (ii) we consider graph G and its closed walks between vertices starting and terminating at v, or w. On the other hand, in item (iii) we considerer only the walks in subgraphs G_v and G_w, respectively. Also, the walks from item (ii) can revisit vertex v (or w); on the other hand, the walks from item (iii), if imbedded in G and extended with the vertex v (resp. w) and appropriate edges can revisit v only once (in the last step). So items (ii) and (iii) are counting different walks.

(iii) Spectral radius of a graph: In Corollary 2.3 we have already given two formulas involving spectral radius. Now for any simple graph G of radius ρ in the right hand side we have essentially to count the number of walks of fixed lengths which start and terminate in the vertices from U (see (9) and (10)). So (9) is reduced to

$$\rho = \sum_{k=0}^{\infty} \frac{W_k(U; G_u)}{\rho^{k+1}}, \tag{17}$$

or to

$$\rho = \sum_{k=0}^{\infty} \frac{W_{2k}(U; G_u)}{\rho^{2k+1}} \tag{18}$$

if G is bipartite.

Remark 3.3. *A particular case of this formula when u is a dominating vertex in G has been shown to the third author by his former students Vladimir Božin and Vladimir Baltić (the proof given here is the original one).*

In what follows we offer some examples in which formula (17) is used.

Let H be the (disjoint) union of k not necessarily equal r-regular graphs H_i ($i = 1, 2, \ldots, k$). So $H = H_1 \cup H_2 \cup \cdots \cup H_k$. Next, let G be the conus over H, that is, $G = K_1 \nabla H$ (here ∇ stand for the join or direct sum of two graphs). Denote by ρ the spectral radius of G. By (17), observing that that $W_n(V(H); H) = \sum_{j=1}^{k} W_n(V(H_j); H)$, where $n_j = |V(H_j)|$ and $W_n(V(H_j); H) = n_j r^n$, (cf. (15)). Therefore, it easily follows that

$$\rho = \frac{r + \sqrt{r^2 + 4h}}{2},$$

where $h = n_1 + \cdots + n_k$. At this place we can add some comments. First for $r = 0$ the corresponding graph G is a star with h legs and we obtain the expected result; for $r = 1$ G is a friend-ship graph and then we also get an expected formula. On the other hand, for $r \geq 3$ we have that components of H (so H_i's) can be of different orders and structures, but the spectral radius of H has always the same value. That means that we can generate arbitrarily large families of graphs with the same spectral radius which does not depend on structures of H_i's.

Assume now that $H = K_{p,q}$ is a complete bipartite graph, and let G be a bipartite graph obtained from H by adding to it a vertex v of degree r ($1 \leq r \leq p$) which belongs to a (colour) class of cardinality q and has r neighbours in another class of cardinality p. Then $W_{2k}(U; H) = r(qp)^{k-1}(qr)$ since we can start in U in one of

r vertices and terminate in U also in one of r vertices. Using (10) we immediately obtain that the spectral radius of G is

$$\rho = \sqrt{pq + \frac{r^2}{p}}.$$

Clearly, if $r = p$ then G is a complete bipartite graph and then we obtain the well-known result from the literature. Otherwise, if $p = q$ and $1 \leq r \leq p$ then, according to [4], the corresponding graph G features as a graph with maximal spectral radius among bipartite graphs with prescribed number of edges. Needless to add the same result can be obtained by the divisor technique (see, for example, [6]), but with more efforts.

Finally, it is worth noting that the following implication holds for two connected graphs G and H with respect to their vertices v and w:

$$\text{if } \mathcal{W}(U_H; H_v) \leq \mathcal{W}(U_G; G_w) \text{ component-wise, then } \rho(H) \leq \rho(G).$$

The most simple example arises if we take that H is any subgraph of G.

(iv) A comment on one of Schwenk formulas: Recall, one of the most exploited Schwenk formula reads:

$$\Phi(x; G) = x\Phi(x; G - v) - \sum_{w \sim v} \Phi(x; G - v - w) - 2 \sum_{C \in \mathcal{C}(v)} \Phi(x; G - V(C)), \tag{19}$$

where $\mathcal{C}(v)$ is the set of all cycles of G passing through vertex v. Using the above observations (see item **(i)**) we can put it in the following form

$$\Phi(x; G) = x\Phi(x; G - v)[1 - g(x; U)], \tag{20}$$

where x is enough small. Needless to add we also have that

$$x\Phi(x; G - v)g(x; U) = \sum_{w \sim v} \Phi(x; G - v - w) + 2 \sum_{C \in \mathcal{C}(v)} \Phi(x; G - V(C)). \tag{21}$$

4. Some Experimental Results

In order to get some impression of how our formula (9) "sounds" in practice we provide some experimental results obtained by a simple program written in Wolfram Mathematica.

Example 4.1. *Let G be a (pseudo)-random graph of order $n = 8$ and size $m = 16$. For each of its one-vertex deleted subgraphs we have calculated the partial sums (up to 65-th term) in order to see how far are they from $\rho = 4.2141907412$, the numeric value of the spectral radius of G with 10 significant digits after decimal point. These results are summarized in Table 1.*

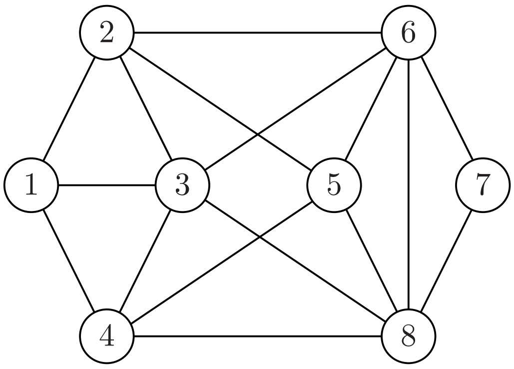

Figure 1: The graph G of Example 4.1.

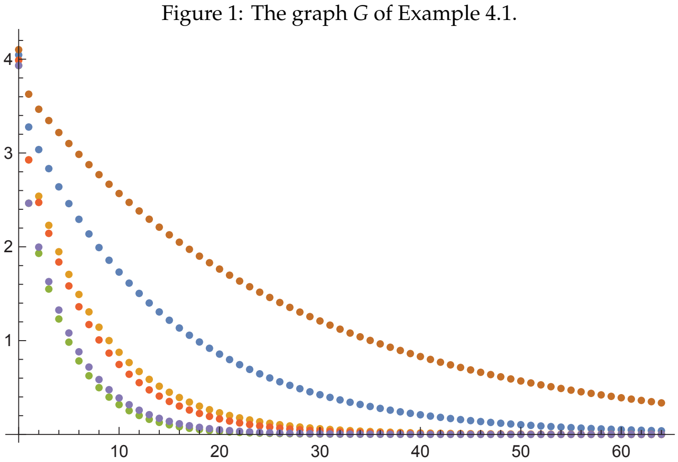

Figure 2: The diagram for Example 4.1.

Table 1: Table for Example 4.1.

vertex deleted subgraph	*partial sums of the RHS of (17)*	*relative errors in %*
G_1	4.17549	0.918336
G_2	4.21354	0.015522
G_3	4.21419	0.000038
G_4	4.21354	0.015522
G_5	4.21397	0.005233
G_6	4.21418	0.000147
G_7	3.87786	7.980980
G_8	4.21418	0.000147

We first observe that vertices 2 *and* 4*, and also* 6 *and* 8*, as expected (due to symmetry), have the same features. This can be seen from the data provided in the table, and also in Fig. 4.1. We can next see that the convergence (of* ρ*) is the fastest with vertex* 3*, and the slowest with vertex* 7*. Vertices* 2*,* 4 *and* 5 *(and also* 3*,* 6 *and* 8*) have the same degrees* 5 *(resp.* 4*) but very close rates of convergence (of* ρ*). In Fig. 2 the dynamics in changing of partial sums for* ρ *is pointed in more details.*

In our forthcoming papers we will examine the phenomena about our formulas with more details.

5. Conclusion

The main results from Section 2, in view of Section 3, seems to be not so much applicable for solving some challenging problems in the spectral graph theory. For example, except some well-known results on the spectral radius we haven't found so far an attractive result that can be obtained by making use of a final note from item **(iii)** in Section 3. Needless to add it is still a big challenge to find some more interesting and also more non-trivial applications of our new formulas from Section 2.

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