

Pacific Journal of Mathematics

THE SPECTRAL APPROACH TO DETERMINING THE NUMBER OF WALKS IN A GRAPH

FRANK HARARY AND ALLEN JOHN CARL SCHWENK

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*Dedicated to Paul Erdős on his sixtieth birthday, and may
 he long continue his academic random walks.*

It is well known that the number of closed walks of length n is simply the n th moment of the adjacency matrix. We find similar spectral expressions for unrestricted (either open or closed) walks, and also for walks from any specified starting set of points to another set of terminal points. Knowledge of the number of walks in G may be applied to find the spectrum of the complement of G . In conclusion, cyclic and dihedral equivalence relations are defined for closed walks and Burnside's lemma is used to enumerate the number of equivalence classes of both types.

The characteristic polynomial of a graph G is defined as that of its adjacency matrix $A(G)$, and we denote it by

$$(1) \quad \phi(G; x) = \prod_{i=1}^p (x - \lambda_i).$$

Since A is real and symmetric, it has only real roots. This sequence of roots $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p$ is called the *spectrum* of G . Another consequence of the symmetry of A is that there exists a unitary matrix that transforms A into Jordan canonical form, and consequently, this form must be a diagonal matrix. Therefore, the minimum polynomial of A can possess no multiple roots, and we write it

$$(2) \quad \mu(G; x) = \prod_{i=1}^d (x - \mu_i) = \sum_{k=0}^d b_k x^k$$

where the μ_i are the distinct roots of (1).

An elementary graph theoretic interpretation identifies the trace of A^n as the number of closed walks of length n in G . But a standard matrix result equates $\text{tr } A^n$ to the n th moment of A defined as

$$(3) \quad M_n(A) = \sum_{i=1}^p \lambda_i^n.$$

Thus, we have found that the number of closed walks of length n in G is simply the sum of the n th powers of the eigenvalues. We might hope that a similar spectral expression could be found for W_n , the number of arbitrary (either open or closed) walks as length

n in G , and this has been done by Cvetković [2]. We proceed to sketch his results. Since A satisfies $\mu(G; x) = 0$, we find for $n \geq d$,

$$(4) \quad A^{n-d} \sum b_k A^k = \sum b_k A^{n-d+k} = 0.$$

Now W_{n-d+k} is simply the sum of the entries in A^{n-d+k} , so summing entries throughout this matrix equation yields

$$(5) \quad \sum_{k=0}^d b_k W_{n-d+k} = 0.$$

This is a linear homogeneous recurrence relation for the number of walks. But notice that for $1 \leq i \leq d$, we may substitute μ_i^j for W_j to obtain a solution to (5) because μ_i satisfies $\mu(G; x) = 0$. Since this provides d particular solutions which are linearly independent, a general solution must be a linear combination of these solutions. That is, W_n must satisfy

$$(6) \quad W_n = \sum_{i=1}^d c_i \mu_i^n$$

where the constants c_i are determined by the initial conditions. Cvetković [2] defined the *main part of the spectrum*, denoted $M = \{\nu_1, \nu_2, \dots, \nu_m\}$ as the set of those distinct eigenvalues which occur in (6) with a nonzero coefficient. For convenience, we relabel the constants in (6), omitting those constants which are 0, to obtain

$$(7) \quad W_n = \sum_{i=1}^m c_i \nu_i^n.$$

Thus, Cvetković laid the groundwork for solving this problem, but he did not describe how M and the constants c_i can be efficiently determined. To do this, we begin by characterizing the main part of the spectrum.

THEOREM 1.2. *The following statements are equivalent for a graph G .*

- (1) $M = \{\nu_1, \nu_2, \dots, \nu_m\}$ is the main part of the spectrum.
- (2) M is the minimum set of eigenvalues the span of whose eigenvectors includes the vector $\beta = (1, 1, \dots, 1)$.
- (3) M is the set of those eigenvalues which have an eigenvector not orthogonal to $\beta = (1, 1, \dots, 1)$.

Proof. (1) is equivalent to (2). Since the eigenvectors of G form a basis for E_p , euclidean p -space, β can be represented as a linear combination of eigenvectors. For multiple eigenvalues, there is some freedom in choosing the eigenvectors, but we may assume they have been chosen so that at most one vector from each multi-

ple set is not orthogonal to β . Consequently, β can be expressed as a linear combination of eigenvectors with distinct eigenvalues and nonzero coefficients, say

$$(8) \quad \beta = \sum_{i=1}^k a_i \alpha_i .$$

Assuming α_i has eigenvalue σ_i , we observe that

$$(9) \quad W_n = A^n \beta \cdot \beta = \sum_{i=1}^k a_i^2 (\alpha_i \cdot \alpha_i) \sigma_i^n .$$

But we have already found the unique expression (7) of this type for W_n , so we conclude that $k = m$ and $M = \{\sigma_1, \sigma_2, \dots, \sigma_k\}$ and that the corresponding constants in (7) and (9) are identical. Thus statements (1) and (2) define the same set, and so (1) is equivalent to (2).

(2) is equivalent to (3). Suppose $\beta = \sum_{i=1}^m a_i \alpha_i$. Then for $1 \leq i \leq m$, $\beta \cdot \alpha_i = a_i (\alpha_i \cdot \alpha_i) \neq 0$, and so every $\nu \in M$ has an eigenvector not orthogonal to β . Conversely, if each eigenvector γ for eigenvalue ν does not appear among the α_i 's, then $\beta \cdot \gamma = \sum a_i \alpha_i \cdot \gamma = 0$. Therefore $\nu \notin M$ implies that all eigenvectors of ν are orthogonal to β , so (2) is equivalent to (3).

Let the neighborhood of v , denoted $N(v)$, be the set of points adjacent to v . In [5, § 3] we call a partition $V_1 \cup V_2 \cup \dots \cup V_m$ of the points of graph G equitable if for all i, j and for all $u, v \in V_i$

$$(10) \quad |N(u) \cap V_j| = |N(v) \cap V_j| .$$

For example, the similarity classes of points formed by the automorphism group of G constitute an equitable partition. We associate with each equitable partition a matrix T defined by

$$(11) \quad t_{ij} = |N(u) \cap V_j|$$

where $u \in V_i$. We conjecture that there is a fourth statement equivalent to the three in Theorem 1.

Conjecture (4). Let the matrix T be obtained from an equitable partition of smallest size. Then T is an $m \times m$ matrix and M is just the set of eigenvalues of T .

If $\alpha_1, \alpha_2, \dots, \alpha_p$ form an orthonormal basis, the theorem permits us to rewrite (7) in the form

$$(12) \quad W_n = \sum_{i=1}^p (\beta \cdot \alpha_i)^2 \lambda_i^n .$$

That is, $\lambda_i \in M$ if and only if $\beta \cdot \alpha_i \neq 0$, and so the constants c_i of (7) are just the squares of the dot products $(\beta \cdot \alpha_i)$.

It is easy to see how to adjust (9) to obtain the number of walks of length n from any subset B of possible starting points to a second subset C of permitted terminal points. Let γ be the vector whose v_i component is 1 or 0 according as v_i is or is not in B . Let δ be the corresponding vector determined by C .

COROLLARY 1a. *The number $W_n(B, C)$ of walks of length n from any set B to another set C is*

$$(13) \quad W_n(B, C) = A^n \gamma \cdot \delta = \sum_{i=1}^p (\gamma \cdot \alpha_i)(\delta \cdot \alpha_i) \lambda_i^n.$$

Since it is well known (see for example Collatz and Sinogowitz [1]) that the largest eigenvalue λ_1 (also called the *spectral radius*) has a nonnegative eigenvector, we see that $c_1 = (\beta \cdot \alpha_1)^2 > 0$, and we quickly obtain another result of Cvetković [3].

THEOREM 2. *The spectral radius is given by*

$$(14) \quad \lambda_1 = \lim_{n \rightarrow \infty} \sqrt[n]{W_n/p}.$$

Notice that since p remains fixed as n increases, it has no affect on the limit. It has been included simply to make the individual terms identical to the n th root of what Cvetković calls “the dynamic average degree”. In particular when $n = 1$, notice that W_n/p is just the usual average degree.

In [5] we discussed the relation between spectra and various graphical operations. We can now determine $\phi(\bar{G})$ and hence the spectrum of the complement. The ordinary generating function for the number of walks of length n is readily found from (7) to be

$$(15) \quad W(x) = \sum_{n=0}^{\infty} W_n x^n = \sum_{i=1}^m c_i / (1 - \nu_i x).$$

Using this function, Cvetković [2] was able to express the characteristic polynomial of the complement in terms of $\phi(G)$.

THEOREM 3. *The characteristic polynomial of \bar{G} is*

$$(16) \quad \phi(\bar{G}; x) = (-1)^p \phi(G; -1-x)(1 - W(-1/(1+x)) / (1+x)).$$

For example, if G is regular, $W(x)$ has the particularly simple form

$$(17) \quad W(x) = p / (1 - rx).$$

Substituting this into (16), we find that for a regular graph G ,

$$(18) \quad \phi(\bar{G}; x) = (-1)^p \phi(G; -1-x)(1+r-p+x)/(1+r+x).$$

By inspection, we see that if $(r, \lambda_2, \lambda_3, \dots, \lambda_p)$ is the spectrum of G , then the spectrum of \bar{G} is $(p-1-r, -1-\lambda_2, -1-\lambda_3, \dots, -1-\lambda_p)$. Notice that most of the eigenvalues are -1 minus the corresponding eigenvalue of G . This is in fact a special case of the following result.

THEOREM 4. *Let α be an eigenvector of G with eigenvalue λ and suppose α is orthogonal to $\beta = (1, 1, \dots, 1)$. Then α is an eigenvector of \bar{G} with eigenvalue $-1 - \lambda$.*

Proof. Since $\bar{A} = J - I - A$, we see that

$$(19) \quad \bar{A}\alpha = J\alpha - I\alpha - A\alpha = 0\alpha - \alpha - \lambda\alpha = (-1 - \lambda)\alpha.$$

In other words, the nonmain eigenvalues of \bar{G} are easily found from those of G . The difficulty is to find the main eigenvalues. Theorem 3 accomplishes this in general. If the Conjecture (4) holds, there is another way to find the main part of the spectrum of \bar{G} . Namely, the equitable partition found for G is also equitable for \bar{G} . The corresponding matrix \bar{T} is given by

$$(20) \quad \bar{t}_{ij} = |V_j| - t_{ij} - \delta_{ij},$$

where δ_{ij} is the Kroneker delta function. Thus, the main eigenvalues are the roots of \bar{T} and the nonmain eigenvalues are readily found from Theorem 4.

We conclude by returning to the enumeration of closed walks. Each walk counted by (3) has a specified starting point. Thus the walks $v_1 v_2 \dots v_{n-1} v_n v_1$ and $v_2 v_3 \dots v_n v_1 v_2$ are different walks (even though they traverse the same points in the same relative order) because one starts at v_1 and the other starts at v_2 . We define two closed walks to be *cyclic equivalent* if one can be obtained from the other by rotating an initial segment to the end of the walk. One might first suspect that each equivalence class has n walks in it, but that is not always true. For example, with $n = 6$, the equivalence class of $v_1 v_2 v_3 v_1 v_2 v_3 v_1$ has just three walks. Thus, we ask what is $C_n(G)$, the number of cyclic equivalence classes of closed walks of length n in G ? Let $\phi(n)$ denote the Euler phi-function¹ and let (i, n) be the greatest common divisor of i and n .

THEOREM 5. $C_n(G) = 1/n \sum_{d|n} \phi(n/d) \sum_{j=1}^n \lambda_j^d.$

Proof. We apply Burnside's lemma (see [4, p. 181]) to the

¹This is a minor sin of notation since $\phi(G; x)$ is the characteristic polynomial.

cyclic group of order n acting on closed walks of length n , observing that a walk W is “fixed” under a rotation of i positions if and only if W consists of a closed walk of length (i, n) repeated $n/(i, n)$ times. Thus

$$(21) \quad C_n(G) = \frac{1}{n} \sum_{i=1}^n \text{tr } A^{(i, n)} .$$

If we let $d = (i, n)$, we may regroup (21) as a sum over the divisors of n . Each d occurs as an exponent as often as it is the greatest common divisor of n and some i , which is just $\phi(n/d)$ times. Therefore,

$$(22) \quad C_n(G) = \frac{1}{n} \sum_{d|n} \phi(n/d) \text{tr } A^d ,$$

and the theorem is verified by substitution from (3).

Another equivalence relation, called *dihedral equivalence*, is obtained if we permit reversals in addition to rotations. That is, we consider the dihedral group D_n acting on closed walks of length n . We let $D_n(G)$ denote the number of these dihedral equivalence classes.

COROLLARY 5a.

$$(23) \quad D_n(G) = \begin{cases} \frac{1}{2n} \sum_{d|n} \phi(n/d) \sum_{j=1}^p \lambda_j^d & \text{if } n \text{ is odd} \\ \frac{1}{2n} \sum_{d|n} \phi(n/d) \sum_{j=1}^p \lambda_j^d + \frac{1}{4} \sum_{j=1}^m c_j \nu_j^{n/2} & \text{if } n \text{ is even} . \end{cases}$$

Proof. The rotations in D_n are handled just as they were in C_n above, so we need only account for the n reflections in D_n . A reflection that interchanges two consecutive points in the walk cannot fix *any* closed walk because two consecutive points must be distinct since G has no loops. But when n is odd, each reflection does interchange two adjacent points, and so we obtain the first half of (23). When n is even, on the other hand, $n/2$ reflections interchange consecutive points while the other $n/2$ reflections do not. These latter reflections “fix” a walk if and only if it consists of an arbitrary walk of length $n/2$ followed by its reversal. Thus, the reflections contribute $n/2(1/2n)W_{n/2}$ when n is even, and so (23) is verified.

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Received March 25, 1976. Research supported in part by grant 73-2502 from the Air Force Office of Scientific Research.

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The *Pacific Journal of Mathematics* is issued monthly as of January 1966. Regular subscription rate: \$72.00 a year (6 Vols., 12 issues). Special rate: \$36.00 a year to individual members of supporting institutions.

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PUBLISHED BY PACIFIC JOURNAL OF MATHEMATICS, A NON-PROFIT CORPORATION

Printed at Kokusai Bunken Insatsusha (International Academic Printing Co., Ltd.).
8-8, 3-chome, Takadanobaba, Shinjuku-ku, Tokyo 160, Japan.

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