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

\[
\phi(G; x) = \prod_{i=1}^{p} (x - \lambda_{i}).
\]

Since \( A \) is real and symmetric, it has only real roots. This sequence of roots \( \lambda_{1} \geq \lambda_{2} \geq \cdots \geq \lambda_{p} \) 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

\[
\mu(G; x) = \prod_{i=1}^{d} (x - \mu_{i}) = \sum_{k=0}^{d} b_k x^k
\]

where the \( \mu_i \) 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

\[
M_n(A) = \sum_{i=1}^{p} \lambda_{i}^{n}.
\]

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
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 $n \geq d$,

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

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

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

This is a linear homogeneous recurrence relation for the number of walks. But notice that for $1 \leq i \leq d$, we may substitute $\mu_i$ for $W_i$ to obtain a solution to (5) because $\mu_i$ 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

$$W_n = \sum_{i=1}^{d} c_i \mu_i^n$$

where the constants $c_i$ are determined by the initial conditions. Cvetković [2] defined the main part of the spectrum, denoted $M = \{\nu_1, \nu_2, \ldots, \nu_m\}$ 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

$$W_n = \sum_{i=1}^{m} c_i \nu_i^n.$$  

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) $M = \{\nu_1, \nu_2, \ldots, \nu_m\}$ is the main part of the spectrum.

(2) $M$ is the minimum set of eigenvalues the span of whose eigenvectors includes the vector $\beta = (1, 1, \ldots, 1)$.

(3) $M$ is the set of those eigenvalues which have an eigenvector not orthogonal to $\beta = (1, 1, \ldots, 1)$.

**Proof.** (1) is equivalent to (2). Since the eigenvectors of $G$ form a basis for $E_\nu$, euclidean $p$-space, $\beta$ 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 $\beta$. Consequently, $\beta$ can be expressed as a linear combination of eigenvectors with distinct eigenvalues and nonzero coefficients, say

\begin{equation}
\beta = \sum_{i=1}^{k} a_i \alpha_i.
\end{equation}

Assuming $\alpha_i$ has eigenvalue $\sigma_i$, we observe that

\begin{equation}
W_n = A^n \beta = \sum_{i=1}^{k} a_i^2 (\alpha_i \cdot \alpha_i) \sigma_i^n.
\end{equation}

But we have already found the unique expression (7) of this type for $W_n$, so we conclude that $k = m$ and $M = \{\sigma_1, \sigma_2, \ldots, \sigma_k\}$ 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 $\beta$. Conversely, if each eigenvector $\gamma$ for eigenvalue $\nu$ does not appear among the $\alpha_i$'s, then $\beta \cdot \gamma = \sum a_i \alpha_i \cdot \gamma = 0$. Therefore $\nu \in M$ implies that all eigenvectors of $\nu$ are orthogonal to $\beta$, 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 $V_1 \cup V_2 \cup \cdots \cup V_m$ of the points of graph $G$ equitable if for all $i, j$ and for all $u, v \in V_i$

\begin{equation}
|N(u) \cap V_j| = |N(v) \cap V_j|.
\end{equation}

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

\begin{equation}
t_{ij} = |N(u) \cap V_j|
\end{equation}

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 $\alpha_1, \alpha_2, \ldots, \alpha_n$ form an orthonormal basis, the theorem permits us to rewrite (7) in the form

\begin{equation}
W_n = \sum_{i=1}^{n} (\beta \cdot \alpha_i)^2 \lambda_i^n.
\end{equation}

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 \( \gamma \) be the vector whose \( v_i \) component is 1 or 0 according as \( v_i \) is or is not in \( B \). Let \( \delta \) 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

\[
W_n(B, C) = A^n \gamma \cdot \delta = \sum_{i=1}^{s} (\gamma \cdot \alpha_i)(\delta \cdot \alpha_i) \lambda_i^n.
\]

Since it is well known (see for example Collatz and Sinogowitz [1]) that the largest eigenvalue \( \lambda_1 \) (also called the spectral radius) has a nonnegative eigenvector, we see that \( c_1 = (\beta \cdot \alpha_i)^2 > 0 \), and we quickly obtain another result of Cvetković [3].

**Theorem 2.** The spectral radius is given by

\[
\lambda_1 = \lim_{n \to \infty} \sqrt[n]{W_n/p}.
\]

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 \( \phi(G) \) 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

\[
W(x) = \sum_{n=0}^{\infty} W_n x^n = \sum_{i=1}^{s} c_i/(1 - \nu_i x).
\]

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

\[
\phi(\bar{G}; x) = (-1)^s \phi(G; -1-x)(1 - W(-1/(1+x))/(1+x)).
\]

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

\[
W(x) = p/(1 - rx).
\]

Substituting this into (16), we find that for a regular graph \( G \),
By inspection, we see that if \((r, \lambda_2, \lambda_3, \ldots, \lambda_p)\) is the spectrum of \(G\), then the spectrum of \(\bar{G}\) is \((p-1-r, -1-\lambda_2, -1-\lambda_3, \ldots, -1-\lambda_p)\). 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 \(\alpha\) be an eigenvector of \(G\) with eigenvalue \(\lambda\) and suppose \(\alpha\) is orthogonal to \(\beta = (1, 1, \cdots, 1)\). Then \(\alpha\) is an eigenvector of \(\bar{G}\) with eigenvalue \(-1-\lambda\).

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

\[
\bar{A}\alpha = J\alpha - I\alpha - A\alpha = 0\alpha - \alpha - \lambda\alpha = (-1 - \lambda)\alpha.
\]

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

\[
\bar{t}_{i\ell} = |V_j| - t_{i\ell} - \delta_{i\ell},
\]

where \(\delta_{i\ell}\) 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 \(v_1v_2\cdots v_nv_1\) and \(v_2v_3\cdots v_nv_1v_2\) 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 \(v_1v_2v_3v_4v_5v_6\) 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-function\(^1\) and let \((i, n)\) be the greatest common divisor of \(i\) and \(n\).

**Theorem 5.** \(C_n(G) = 1/n \sum_{d|n} \phi(n/d) \sum_{j=1}^{\lambda_d} \lambda_d^j\).

**Proof.** We apply Burnside’s lemma (see [4, p. 181]) to the  
\(^1\)This 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

\[
C_n(G) = \frac{1}{n} \sum_{i=1}^{n} \text{tr} A^{(i, n)}.
\]

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,

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

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.**

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

**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.

**References**


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