Number of Walks and Degree Powers in a Graph *

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April 26, 2006

Abstract

This letter deals with the relationship between the total number of k-walks in a graph, and the sum of the k-th powers of its vertex degrees. In particular, it is shown that the sum of all k-walks is upper bounded by the sum of the k-th powers of the degrees.

Let $G = (V, E)$ be a connected graph on n vertices, $V = \{1, 2, \dots, n\}$, with adjacency matrix $\boldsymbol{A}$. For any integer $k \geq 1$, let $a_{ij}^{(k)}$ denote the (i, j) entry of the power matrix $\boldsymbol{A}^k$. Let $\boldsymbol{D}$ be the diagonal matrix with elements $(\boldsymbol{D})_{ii} = d_i$ (the degree of vertex i). Here we study the relationship between the sum of all walks of length k in G and the sum of the k-th powers of its degrees. As a main result, and answering in the affirmative a conjecture of Marc Noy [8], we will show that

$$\sum_{i,j} a_{ij}^{(k)} \leq \sum_i d_i^k, \tag{1}$$

with equality if and only if G is regular or $k \leq 2$. In the case $k = 3$ we also provide an exact value of the difference between the above sums in (1). In other line of research, some upper bounds for $\sum_i d_i^k$ have been given by several authors. See, for instance, [7, 9, 6, 4] (for general graphs) and [3, 2] (for graphs not containing a prescribed subgraph).

Let us first begin with the small values of k. The case $k = 0$ is trivial since the number of walks of length 0 equals the number of vertices. Similarly, if $k = 1$, the sum $\sum_{i,j} a_{ij}$ is just the sum of the degrees $d_1 + d_2 + \cdots + d_n$. If $k = 2$, we can use that $\boldsymbol{Aj} = \boldsymbol{Dj}$ (where $\boldsymbol{j}$ is the all-1 vector) and the symmetry of the involved matrices to obtain:

$$\sum_{i,j} a_{ij}^{(2)} = \langle \boldsymbol{j}, \boldsymbol{A}^2\boldsymbol{j} \rangle = \langle \boldsymbol{Aj}, \boldsymbol{Aj} \rangle = \|\boldsymbol{Aj}\|^2 = \|\boldsymbol{Dj}\|^2 = d_1^2 + d_2^2 + \cdots + d_n^2.$$

*Work supported by *MEC* and *DURSI* under projects MTM2005-08990-C02-01 and SGR2005-00412.

Assume now that G is regular of degree, say, d. Then, $\boldsymbol{j}$ is the positive eigenvector corresponding to the eigenvalue d and we get

$$\langle \boldsymbol{j}, \boldsymbol{A}^k \boldsymbol{j}\rangle = \langle \boldsymbol{j}, d^k \boldsymbol{j}\rangle = d^k \|\boldsymbol{j}\|^2 = nd^k.$$

A similar reasoning shows that, for a general (non-regular) graph, the inequality in (1) always holds for k large enough. Indeed, let $\boldsymbol{\nu}$ be the positive eigenvector of G, normalized in such a way that $\min_{i\in V} \nu_i = 1$. Let λ be its corresponding (positive) eigenvalue, which is known to be smaller than the maximum degree Δ of G (see [1, 5]). Then,

$$\langle \boldsymbol{\nu}, \boldsymbol{A}^k \boldsymbol{\nu}\rangle = \langle \boldsymbol{\nu}, \lambda^k \boldsymbol{\nu}\rangle = \|\boldsymbol{\nu}\|^2 \lambda^k$$

which, for k large enough, is smaller than the single k-power Δ^k.

To deal with the case $k = 3$, it is more convenient to work with the Laplacian matrix of G; that is, $\boldsymbol{L} := \boldsymbol{D} - \boldsymbol{A}$. Then, recall that, given any real function defined on V, $f : V \to \mathbb{R}$, and with $\boldsymbol{f}$ being the (column) vector with components the values of f on V, we have

$$\langle \boldsymbol{f}, \boldsymbol{L}\boldsymbol{f}\rangle = \sum_{i\sim j} (f(i) - f(j))^2,$$

where the sum is extended over all edges of G (see, for instance, [1]). We are interested in the case when the above function is just the degree of the corresponding vertex: $f(i) = d_i$. In this case, we denote by $\boldsymbol{\delta}$ its corresponding vector. Then, the difference between the two sums in (1) is just

$$\langle \boldsymbol{\delta}, \boldsymbol{L}\boldsymbol{\delta}\rangle = \sum_{i\sim j} [d_i - d_j]^2 \geq 0.$$

To prove the inequality in the general case, note first that, for any two positive numbers a, b with, say, $a \geq b$,

$$a^r b + ab^r = a^{r+1} + b^{r+1} - (a^r - b^r)(a - b) \leq a^{r+1} + b^{r+1}.$$

with equality if and only if $a = b$. (The same conclusion is reached when we apply the Cauchy-Schwarz inequality to the vectors (a^r, a) and (b, b^r).)

Also, notice that all walks of a given length, say $k \geq 1$, can be obtained by considering, for any vertex i, all (i, j)-walks of length $k - 1$ "extended" by each of the d_i edges incident to i. Thus, $\sum_{i,j} a_{ij}^{(k)} = \sum_{i,j} d_i a_{ij}^{(k-1)}$ or, equivalently,

$$\langle \boldsymbol{j}, \boldsymbol{A}^k \boldsymbol{j}\rangle = \langle \boldsymbol{j}, \boldsymbol{A}^{k-1} \boldsymbol{D}\boldsymbol{j}\rangle = \langle \boldsymbol{D}\boldsymbol{j}, \boldsymbol{A}^{k-1} \boldsymbol{j}\rangle.$$

Keeping all this in mind, we are now ready to prove (1). Indeed, assuming that $k \geq 3$, we have:

$$\begin{aligned}
\sum_{i,j} a_{ij}^{(k)} &= \sum_{i,j} d_i a_{ij}^{(k-2)} d_j = \sum_i a_{ii}^{(k-2)} d_i^2 + \sum_{i<j} 2a_{ij}^{(k-2)} d_i d_j \\
&\leq \sum_i a_{ii}^{(k-2)} d_i^2 + \sum_{i<j} a_{ij}^{(k-2)} (d_i^2 + d_j^2) \\
&= \sum_{i,j} a_{ij}^{(k-2)} d_j^2 \\
&= \sum_{i,j} d_i a_{ij}^{(k-3)} d_j^2 = \sum_i a_{ii}^{(k-3)} d_i^3 + \sum_{i<j} a_{ij}^{(k-3)} (d_i d_j^2 + d_i^2 d_j) \\
&\leq \sum_i a_{ii}^{(k-3)} d_i^3 + \sum_{i<j} a_{ij}^{(k-3)} (d_i^3 + d_j^3) \\
&= \sum_{i,j} a_{ij}^{(k-3)} d_j^3 \leq \cdots \leq \sum_{i,j} a_{ij} d_j^{k-1} = \sum_j d_j^k.
\end{aligned}$$

Moreover, notice that all the above inequalities become equalities if and only if G is regular, as claimed.

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