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**A note on walk entropies in graphs**

by

Michele Benzi

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**EMORY UNIVERSITY**

# A NOTE ON WALK ENTROPIES IN GRAPHS

MICHELE BENZI*

**Abstract.** The concept of *walk entropy* of a graph has been recently introduced in [E. Estrada, J. A. de la Peña, and N. Hatano, *Walk entropies in graphs*, Linear Algebra Appl., to appear]. In that paper the authors formulated two conjectures about walk entropies. In the present note we prove the first of these two conjectures and propose a stronger form of it.

**Key words.** entropy measures, graph walks, walk-regular graphs

**AMS subject classifications.** 05C50, 15A16, 82C20

**1. Introduction.** The notion of *walk entropy* in a graph, recently introduced by Estrada, de la Peña and Hatano [4], enjoys a number of interesting properties that can be used to characterize and analyze graphs.

For a simple, undirected graph $G = (V, E)$ with $n$ nodes $v_1, \dots, v_n$ and adjacency matrix $A$, the walk entropy of $G$ is defined as

$$S^V(G, \beta) = -\sum_{i=1}^{n} \frac{\left[e^{\beta A}\right]_{ii}}{Z} \ln \frac{\left[e^{\beta A}\right]_{ii}}{Z}, \quad \text{where} \quad Z = \mathrm{Tr}\left[e^{\beta A}\right].$$

Here $\beta > 0$ can be interpreted as an *inverse temperature*. In other words, the walk entropy of $G$ is the Gibbs–Shannon entropy associated with the probability distribution

$$p_i(\beta) = \frac{\left[e^{\beta A}\right]_{ii}}{\mathrm{Tr}\left[e^{\beta A}\right]}, \quad 1 \le i \le n$$

on $V$. As noted in [4], natural logarithms or base 2 ones can be used interchangeably in the definition of $S^V(G, \beta)$ without any significant differences.

Recall that for a given $\beta > 0$, the *subgraph centrality* [7] of a node $v_i \in V$ is given by

$$SC(i, \beta) = [e^{\beta A}]_{ii} = \sum_{k=0}^{\infty} \frac{\beta^k [A^k]_{ii}}{k!}.$$

The subgraph centrality of a node counts the number of closed walks starting and ending at that node, with smaller weights assigned to longer walks (the total number of closed walks of length $k$ is scaled by $\beta^k/k!$). Frequently, the inverse temperature $\beta$ is set equal to 1. Subgraph centrality has been used as an effective measure of the importance of nodes in a network [3, 5]. As with all (reasonable) centrality measures, however, there are graphs for which subgraph centrality does not discriminate between nodes; that is, graphs for which

$$SC(i, \beta) = \frac{1}{n} \mathrm{Tr}\left[e^{\beta A}\right], \quad \forall\, i = 1, \dots, n. \tag{1.1}$$

This is true, for example, for $G = C_n$ (a cycle with $n$ vertices) and, more generally, for all *vertex-transitive* graphs [8]. Recall that a graph $G = (V, E)$ is vertex-transitive

*Department of Mathematics and Computer Science, Emory University, Atlanta, Georgia 30322, USA (benzi@mathcs.emory.edu). The work of this author was supported by National Science Foundation grant DMS-0810862.

if, given any two nodes $u, v \in V$, there exists an automorphism $f_{u,v} : V \to V$ such that $f_{u,v}(u) = v$. Other examples of graphs satisfying (1.1) are mentioned in [4].

We will also need the definition of a *walk-regular* graph [8]. A graph $G = (V, E)$ is walk-regular if for all $k = 0, 1, 2, \ldots$, the diagonal entries of $A^k$ are all equal:

$$\left[A^k\right]_{ii} = c(k)\,, \quad \forall\, i = 1, \ldots, n\,.$$

In particular, walk-regular graphs are regular (all the nodes have the same degree). The name walk-regular originates from the fact that $\left[A^k\right]_{ii}$ equals the number of closed walks of length $k$ in $G$ starting and ending at node $i$. We note that thanks to the Cayley–Hamilton Theorem, it is sufficient that the above conditions hold for all $1 \le k \le n-1$. It is obvious that if a graph is walk-regular, (1.1) must hold; hence, for a walk-regular graph, subgraph centrality does not discriminate between nodes.

It is easy to see that for a given value of $\beta$, the walk entropy $S^V(G, \beta)$ assumes its maximum value when, and only when, all nodes have the same subgraph centrality $SC(i, \beta)$ and that this maximum is given by

$$S^V(G, \beta) = -\sum_{i=1}^{n} \frac{1}{n} \ln \frac{1}{n} = \ln n\,.$$

It follows from the foregoing discussion that for a walk-regular graph, the entropy is maximized. The entropy is also maximized, trivially, when $\beta = 0$, for any graph $G$.

In [4], the authors state the following

CONJECTURE 1.1. *A graph is walk-regular if and only if $S^V(G, \beta) = \ln n$ for all $\beta \ge 0$.*

In this note we give a proof of this statement, and we conjecture that a stronger version of this statement holds true.

**2. Proof of the conjecture.** Below we give a proof of Conjecture 1.1, and we propose a reformulation of it that suggests that a stronger result may be true.

THEOREM 2.1. *A graph $G$ is walk-regular if and only if $S^V(G, \beta) = \ln n$ for all $\beta \ge 0$.*

*Proof.* As noted before, we only need to show that $G$ is walk-regular if $S^V(G, \beta) = \ln n$ for all $\beta > 0$; the latter condition is equivalent to assuming that $SC(i, \beta) = \left[\mathrm{e}^{\beta A}\right]_{ii} = \phi_0(\beta) \equiv \mathrm{Tr}\left[\mathrm{e}^{\beta A}\right]/n$ for all $i = 1, \ldots, n$. Note that $\phi_0(\beta)$ is a real analytic function of $\beta$ and can be expanded in a power series:

$$\phi_0(\beta) = 1 + \frac{\beta^2}{2!} d_i + \frac{\beta^3}{3!}\left[A^3\right]_{ii} + \frac{\beta^4}{4!}\left[A^4\right]_{ii} + \cdots\,, \quad \forall i = 1, \ldots, n, \tag{2.1}$$

where $d_i = \left[A^2\right]_{ii}$ is the degree of the $i$th node in the graph (note that the first order term is missing in (2.1) since $G$ has no loops, hence $[A]_{ii} = 0$ for all $i$). Rearranging (2.1) into

$$d_i + \frac{\beta}{3}\left[A^3\right]_{ii} + \frac{\beta^2}{12}\left[A^4\right]_{ii} + \cdots = \frac{\phi_0(\beta) - 1}{\beta^2} \equiv \phi_1(\beta), \quad \forall i = 1, \ldots, n, \tag{2.2}$$

and taking the limit as $\beta \to 0+$ we find

$$d_i = \lim_{\beta \to 0+} \phi_1(\beta) \equiv d, \quad \forall i = 1, \ldots, n,$$

showing that $G$ is necessarily regular. Next, rearranging (2.2) with $d_i$ replaced by $d$ we obtain

$$\left[A^3\right]_{ii} + \frac{\beta}{4}\left[A^4\right]_{ii} + \cdots = \frac{3(\phi_1(\beta) - d)}{\beta} \equiv \phi_2(\beta), \quad \forall i = 1, \ldots, n, \tag{2.3}$$

and taking the limit as $\beta \to 0+$ we find

$$\left[A^3\right]_{ii} = \lim_{\beta \to 0+} \phi_2(\beta), \quad \forall i = 1, \ldots, n,$$

showing that $A^3$ has constant diagonal entries. It is clear that the process can be continued indefinitely, showing that each $A^k$ has constant diagonal entries for all $k \geq 2$; hence, $G$ is walk-regular. □

We note that the same conclusion holds with slightly different assumptions.

THEOREM 2.2. *A graph is walk-regular if and only if $S^V(G, \beta) = \ln n$ for all $\beta \in I \subseteq \mathbb{R}$, where $I$ is any set of real numbers containing an accumulation point.*

*Proof.* Again, it is obvious that if $G$ is walk-regular then the walk entropy is equal to $\ln n$ regardless of $\beta$. The other direction is a consequence of the Identity Theorem for analytic functions; see. e.g., [9, Chapter 6]. Indeed, the walk entropy $S^V(G, \beta)$, as a function of $\beta$, can be continued analytically to a strip $\mathcal{S}_\delta = \{z = x + \mathrm{i}y \,|\, x \in \mathbb{R},\ |y| < \delta\}$ for some $\delta > 0$. To see this, we need to show that there is a $\delta > 0$ such that the function $p_i(z) = \left[\mathrm{e}^{zA}\right]_{ii} / \mathrm{Tr}\left[\mathrm{e}^{zA}\right]$ is well defined and non-vanishing on $\mathcal{S}_\delta$. Hence, we need to show that neither the numerator (for $i = 1, \ldots, n$) nor the denominator in the fraction expressing $p_i(z)$ can be zero for $z = x + \mathrm{i}y$ when $x \in \mathbb{R}$ and $y$ is sufficiently small. We have

$$\left[\mathrm{e}^{zA}\right]_{ii} = \left[\mathrm{e}^{xA}\mathrm{e}^{\mathrm{i}yA}\right]_{ii} = \left\langle \mathrm{e}^{xA}\,\mathbf{e}_i, \mathrm{e}^{-\mathrm{i}yA}\,\mathbf{e}_i \right\rangle,$$

where $\mathbf{e}_i$ is the $i$th standard basis vector and $\langle \cdot, \cdot \rangle$ denotes the standard inner product in $\mathbb{C}^n$. Note that the matrix $\mathrm{e}^{-\mathrm{i}yA}$ is unitary, and for $y \to 0$ it tends to the identity matrix. Since $\langle \mathrm{e}^{xA}\,\mathbf{e}_i, \mathbf{e}_i \rangle = \left[\mathrm{e}^{xA}\right]_{ii} > 0$, by continuity there is a $\delta_i > 0$ such that $\langle \mathrm{e}^{xA}\,\mathbf{e}_i, \mathrm{e}^{-\mathrm{i}yA}\,\mathbf{e}_i \rangle \neq 0$ for $|y| < \delta_i$; letting $\delta' = \min_i \delta_i$, we have that all the numerators in $p_i(z)$ are nonzero for $z \in \mathcal{S}_{\delta'}$. For the denominator, observe that

$$\mathrm{Tr}\left[\mathrm{e}^{zA}\right] = \mathrm{Tr}\left[\mathrm{e}^{xA}\mathrm{e}^{\mathrm{i}yA}\right] = \langle \mathrm{e}^{xA}, \mathrm{e}^{-\mathrm{i}yA} \rangle_F$$

where $\langle \cdot, \cdot \rangle_F$ denotes the Frobenius inner product in $\mathbb{C}^{n \times n}$; for $y = 0$ the above inner product is just the trace of the symmetric positive definite matrix $\mathrm{e}^{xA}$, hence it is positive. Again by continuity, there is a $\delta'' > 0$ such that $\mathrm{Tr}\left[\mathrm{e}^{zA}\right] \neq 0$ for all $z \in \mathcal{S}_{\delta''}$. Taking $\delta = \min\{\delta', \delta''\}$ we conclude that $p_i(z)$ is well defined and non-vanishing for all $z \in \mathcal{S}_\delta$, therefore $S^V(G, \beta)$ can be continued analytically to $\mathcal{S}_\delta$. Finally, since $S^V(G, z)$ is constant on a set containing an accumulation point, it must be constant everywhere on $\mathcal{S}_\delta$ by the Identity Theorem. In particular, $S^V(G, \beta) = \ln n$ for all $\beta \in \mathbb{R}$. By Theorem 2.1, $G$ must be walk-regular. □

**3. A stronger form of the conjecture.** It follows from Theorem 2.2 that if $S^V(G, \beta) = \ln n$ for all $\beta$ in a real interval of arbitrarily small (but positive) length, then the graph is walk-regular.

We conjecture that the same conclusion holds if the set $I$ reduces to a single real number $\beta \neq 0$.

CONJECTURE 3.1. *A graph is walk-regular if and only if there exists a $\beta \in \mathbb{R}$, $\beta \neq 0$, such that $S^V(G, \beta) = \ln n$.*

Equivalently: If a graph $G$ is not walk-regular, then $S^V(G,\beta) < \ln n$ for all $\beta \neq 0$. In other words, $S^V(G,\beta)$ cannot have more than one global maximum. Note that for a regular graph, $S^V(G,\beta)$ tends asymptotically to $\ln n$ as $\beta \to \infty$, since in this limit the subgraph centralities $SC(i,\beta)$ reduce to (scaled and squared) eigenvector centralities [1], and for a regular graph the dominant eigenvector has constant entries.

For the special case $\beta = 1$, Conjecture 3.1 has been stated by Estrada in [2]. At the time of this writing, it has been verified for all graphs with up to $n = 11$ nodes by computer. We also mention that it is not even known, at this time, if $\left[\mathrm{e}^{\beta A}\right]_{ii} =$ constant (for some $\beta > 0$) implies that $G$ is regular. See also [10, 11] for further discussion of this and related questions.

Note that the falsity of Conjecture 3.1 would imply the existence of graphs for which all the nodes become tied (and thus indistinguishable), in terms of subgraph centrality, for certain isolated, finite values of the "temperature". Moreover any change in the temperature, no matter how small, would break the tie.

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