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# A note on walk entropies in graphs

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ABSTRACT

The concept of *walk entropy* of a graph has been recently introduced in E. Estrada et al. (2014) [4]. 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.



## 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

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

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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

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

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

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

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 [3,5,6]. As with all (reasonable) centrality measures, however, there are graphs for which subgraph centrality does not discriminate between nodes; that is, graphs for which

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

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 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 $[A^k]_{ii}$ 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 $1 \leqslant k \leqslant n - 1$. 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

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