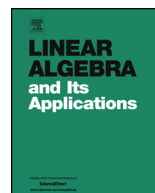




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A note on walk entropies in graphs



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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.

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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

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

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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

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

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 β 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

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

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 $f_{u,v} : V \rightarrow V$ 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 $k = 0, 1, 2, \dots$, the diagonal entries of A^k are all equal

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

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 $1 \leq k \leq n-1$. 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 β , 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

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

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