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Walk entropy and walk-regularity

Kyle Kloster [a,*,1], , Daniel Král' [b,2], Blair D. Sullivan [a,1]

[a] *Department of Computer Science, NC State University, Raleigh, NC 27695, USA*
[b] *Mathematics Institute, DIMAP and Department of Computer Science, University of Warwick, Coventry CV4 7AL, UK*

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ABSTRACT

A graph is said to be walk-regular if, for each $\ell \geq 1$, every vertex is contained in the same number of closed walks of length ℓ. We construct a 24-vertex graph H_4 that is not walk-regular yet has maximized walk entropy, $S^V(H_4, \beta) = \log 24$, for some $\beta > 0$. This graph is a counterexample to a conjecture of Benzi (2014) [1, Conjecture 3.1]. We also show that there exist infinitely many temperatures $\beta_0 > 0$ so that $S^V(G, \beta_0) = \log n_G$ if and only if a graph G is walk-regular.

* Corresponding author.
E-mail addresses: kakloste@ncsu.edu (K. Kloster), d.kral@warwick.ac.uk (D. Král'), blair_sullivan@ncsu.edu (B.D. Sullivan).

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1. Introduction

We study the interplay between the structural property of graphs called walk-regularity and the algebraic property called walk entropy. A simple graph G is *walk-regular* [8] if every vertex of G is contained in the same number of closed walks of length ℓ for every $\ell \in \mathbb{N}$. Observe that a graph G is walk-regular if and only if for every $\ell \in \mathbb{N}$, all the diagonal entries of the power $\boldsymbol{A}^\ell$ of the adjacency matrix $\boldsymbol{A}$ of G are the same. Also note that if a graph G is walk-regular, then it is necessarily degree-regular, i.e., every vertex of G has the same degree.

Estrada et al. [5] initiated the study of the relationship between walk-regularity and an algebraic parameter of a graph called the walk entropy. The *walk entropy* of a graph G at the *temperature* $\beta \geq 0$ is defined as

$$S^V(G,\beta) = -\sum_{i=1}^{n_G} \frac{\left[\mathrm{e}^{\beta \boldsymbol{A}}\right]_{ii}}{\mathrm{Tr}\ \mathrm{e}^{\beta \boldsymbol{A}}} \log \frac{\left[\mathrm{e}^{\beta \boldsymbol{A}}\right]_{ii}}{\mathrm{Tr}\ \mathrm{e}^{\beta \boldsymbol{A}}} ,$$

where n_G denotes the number of vertices of G (in general, we use n_H for the number of vertices of a graph H throughout the paper). In other words, the walk entropy is the entropy associated with the probability distribution on the vertex set $V(G)$ that is linearly proportional to the subgraph centrality of the vertices. We note that any probability distribution on $V(G)$ gives rise to a corresponding notion of graph entropy; Dehmer [3] called such distributions *information functionals*, and introduced this more general class of graph entropies.

The *subgraph centrality* of the i-th vertex of a graph G [7] is equal to $\left[\mathrm{e}^{\beta \boldsymbol{A}}\right]_{ii}$, the corresponding diagonal entry of $\mathrm{e}^{\beta \boldsymbol{A}}$. Note that the walk entropy $S^V(G,\beta) \in [0, \log n_G]$ and $S^V(G,\beta) = \log n_G$ if and only if all the diagonal entries of $\mathrm{e}^{\beta \boldsymbol{A}}$ are the same. That is, walk entropy is maximized precisely when all the vertices have the same subgraph centrality.

It is easy to see that if a graph G is walk-regular, then its walk entropy $S^V(G,\beta)$ is equal to $\log n_G$ for every $\beta \geq 0$. Estrada et al. [5] conjectured that the converse is also true.

Conjecture 1 *(Estrada et al. [5, Conjecture 1]). A graph G is walk-regular if and only if $S^V(G,\beta) = \log n_G$ for all $\beta \geq 0$.*

The conjecture was proven by Benzi in the following stronger form.

Theorem 1 *(Benzi [1, Theorem 2.2]). Let I be any set of real numbers containing an accumulation point. If a graph G satisfies $S^V(G,\beta) = \log n_G$ for all $\beta \in I$, then G is walk-regular.*

Benzi also proposed the following strengthening of his result.