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Walk entropy and walk-regularity

Kyle Kloster*   Daniel Král'†   Blair D. Sullivan*

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 [Linear Algebra Appl. 443 (2014), 395–399, 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.

MSC: 05C50

Keywords: graph entropy; walk-regularity; subgraph centrality; matrix exponential

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

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

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 $\left[e^{\beta A}\right]_{ii}$, the corresponding diagonal entry of $e^{\beta A}$. 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 $e^{\beta A}$ 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.

Conjecture 2 (Benzi [1, Conjecture 3.1]). *A graph G is walk-regular if and only if there exists $\beta > 0$ such that $S^V(G,\beta) = \log n_G$.*

From the contrapositive, Estrada et al. [5,6] proposed that non–degree-regular graphs cannot have maximum walk entropy.

Conjecture 3 (Estrada et al. [6, Conjecture 1.2]). *Let G be a non–degree-regular graph. Then $S^V(G,\beta) < \log n_G$ for every $\beta > 0$.*

Estrada et al. [6] attempted to prove Conjectures 2 and 3, but their argument contains a flaw. In Section 2 we show that Conjectures 2 and 3 are false by presenting a 24-vertex graph, which we denote H_4, that is not walk-regular yet

attains $S^V(H_4, \beta) = \log 24$ for some $\beta > 0$. The graph H_4 contains vertices of degree four and five, i.e., it is not even degree-regular, which resolves the question, mentioned in the concluding remarks in [1], of whether degree-regularity is implied by the existence of a β that maximizes walk entropy. On the positive side, we show that there exist infinitely many temperatures $\beta_0 > 0$ such that a graph G is walk-regular if and only if $S^V(G, \beta_0) = \log n_G$ (Corollary 4), i.e., there are temperatures that properly classify walk-regularity.

2 Non–degree-regular graph maximizing walk entropy

In this section, we present a counterexample to Conjectures 2 and 3. We start by presenting a closed formula for the diagonal entries of the exponential of the adjacency matrix of a graph. Let G be a graph and $\boldsymbol{A}$ its adjacency matrix. Further, let $\lambda_1, \ldots, \lambda_{n_G}$ be the eigenvalues of $\boldsymbol{A}$ and $\mathbf{u}_1, \ldots, \mathbf{u}_{n_G}$ an orthonormal basis formed by the eigenvectors of $\boldsymbol{A}$. It follows that

$$\left[e^{\beta \boldsymbol{A}} \right]_{ii} = \sum_{k=1}^{n_G} \mathbf{u}_{k,i}^2 \cdot e^{\beta \lambda_k} \tag{1}$$

for every $i = 1, \ldots, n_G$. In particular, each diagonal entry of $e^{\beta \boldsymbol{A}}$ is an analytic function of β, which is a linear combination of at most n_G exponential functions.

We next present a construction of graphs H_m parameterized by a positive integer $m \in \mathbb{N}$. The graph H_m is obtained from m isolated vertices and $m + 1$ cliques of order m by including a perfect matching between the m isolated vertices and each of the $m+1$ cliques. The graph H_m has $m+(m+1)m = m^2+2m$ vertices; m vertices have degree $m + 1$ and the remaining $m^2 + m$ vertices have degree m. We are convinced that H_m is a counterexample to Conjecture 2 for every $m \geq 4$; however, we will here analyze the case $m = 4$ only. The graph H_4 and its adjacency matrix are presented in Figure 1.

Theorem 2. *There exists $\beta > 0$ such that $S^V(H_4, \beta) = \log 24$.*

Proof. Let $\boldsymbol{A}$ be the adjacency matrix of the graph H_4. The matrix $\boldsymbol{A}$ has six different eigenvalues, which are given with corresponding eigenvectors in Table 1. Note that the vectors given in Table 1 are not normalized to be unit and orthogonal. We will show that there exists $\beta > 0$ such that all the diagonal entries of the matrix $e^{\beta \boldsymbol{A}}$ are the same, which yields the statement of the theorem.

Let $f_1(\beta) = \left[e^{\beta \boldsymbol{A}} \right]_{11}$ and $f_2(\beta) = \left[e^{\beta \boldsymbol{A}} \right]_{55}$. Note that $\left[e^{\beta \boldsymbol{A}} \right]_{ii} = f_1(\beta)$ for $i = 1, \ldots, 4$ and $\left[e^{\beta \boldsymbol{A}} \right]_{ii} = f_2(\beta)$ for $i = 5, \ldots, 24$. Observe that the k-th derivative of $f_i(\beta)$ for $\beta = 0$ is equal to the corresponding diagonal entry of $\boldsymbol{A}^k$. In particular, $f_1(0) = f_2(0) = 1$, $f_1'(0) = f_2'(0) = 0$, $f_1''(0) = 5$ and $f_2''(0) = 4$. This implies that

3

$$\boldsymbol{A}_{K_4} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}, \boldsymbol{I}_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \boldsymbol{A}_{H_4} = \begin{pmatrix} 0 & \boldsymbol{I}_4 & \boldsymbol{I}_4 & \boldsymbol{I}_4 & \boldsymbol{I}_4 & \boldsymbol{I}_4 \\ \boldsymbol{I}_4 & \boldsymbol{A}_{K_4} & 0 & 0 & 0 & 0 \\ \boldsymbol{I}_4 & 0 & \boldsymbol{A}_{K_4} & 0 & 0 & 0 \\ \boldsymbol{I}_4 & 0 & 0 & \boldsymbol{A}_{K_4} & 0 & 0 \\ \boldsymbol{I}_4 & 0 & 0 & 0 & \boldsymbol{A}_{K_4} & 0 \\ \boldsymbol{I}_4 & 0 & 0 & 0 & 0 & \boldsymbol{A}_{K_4} \end{pmatrix}$$

Figure 1: The graph H_4 and its adjacency matrix $\boldsymbol{A}_{H_4}$.

Eigenvalue	Eigenvector				
$\frac{3+\sqrt{29}}{2} \approx 4.193$	$\left(\frac{10}{3+\sqrt{29}}, \frac{10}{3+\sqrt{29}}, \frac{10}{3+\sqrt{29}}, \frac{10}{3+\sqrt{29}}, \right.$ 1,1,1,1,	1,1,1,1,	1,1,1,1,	1,1,1,1,	1,1,1,1 $\big)$
3	$\big(0,0,0,0,$ 1,1,1,1,	$-1,-1,-1,-1,$	0,0,0,0,	0,0,0,0,	0,0,0,0 $\big)$
3	$\big(0,0,0,0,$ 1,1,1,1,	0,0,0,0,	$-1,-1,-1,-1,$	0,0,0,0,	0,0,0,0 $\big)$
3	$\big(0,0,0,0,$ 1,1,1,1,	0,0,0,0,	0,0,0,0,	$-1,-1,-1,-1,$	0,0,0,0 $\big)$
3	$\big(0,0,0,0,$ 1,1,1,1,	0,0,0,0,	0,0,0,0,	0,0,0,0,	$-1,-1,-1,-1$ $\big)$
$\frac{-1+\sqrt{21}}{2} \approx 1.791$	$\left(\frac{10}{-1+\sqrt{21}}, \frac{-10}{-1+\sqrt{21}}, 0,0, \right.$ $1,-1,0,0,$	$1,-1,0,0,$	$1,-1,0,0,$	$1,-1,0,0,$	$1,-1,0,0$ $\big)$
$\frac{-1+\sqrt{21}}{2} \approx 1.791$	$\left(\frac{10}{-1+\sqrt{21}}, 0, \frac{-10}{-1+\sqrt{21}}, 0, \right.$ $1,0,-1,0,$	$1,0,-1,0,$	$1,0,-1,0,$	$1,0,-1,0,$	$1,0,-1,0$ $\big)$
$\frac{-1+\sqrt{21}}{2} \approx 1.791$	$\left(\frac{10}{-1+\sqrt{21}}, 0,0, \frac{-10}{-1+\sqrt{21}}, \right.$ $1,0,0,-1,$	$1,0,0,-1,$	$1,0,0,-1,$	$1,0,0,-1,$	$1,0,0,-1$ $\big)$
-1	$\big(0,0,0,0,$ $1,-1,0,0,$	$-1,1,0,0,$	0,0,0,0,	0,0,0,0,	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,0,-1,0,$	$-1,0,1,0,$	0,0,0,0,	0,0,0,0,	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,0,0,-1,$	$-1,0,0,1,$	0,0,0,0,	0,0,0,0,	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,-1,0,0,$	0,0,0,0,	$-1,1,0,0,$	0,0,0,0,	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,0,-1,0,$	0,0,0,0,	$-1,0,1,0,$	0,0,0,0,	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,0,0,-1,$	0,0,0,0,	$-1,0,0,1,$	0,0,0,0,	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,-1,0,0,$	0,0,0,0,	0,0,0,0,	$-1,1,0,0,$	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,0,-1,0,$	0,0,0,0,	0,0,0,0,	$-1,0,1,0,$	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,0,0,-1,$	0,0,0,0,	0,0,0,0,	$-1,0,0,1,$	0,0,0,0 $\big)$
-1	$\big(0,0,0,0,$ $1,-1,0,0,$	0,0,0,0,	0,0,0,0,	0,0,0,0,	$-1,1,0,0$ $\big)$
-1	$\big(0,0,0,0,$ $1,0,-1,0,$	0,0,0,0,	0,0,0,0,	0,0,0,0,	$-1,0,1,0$ $\big)$
-1	$\big(0,0,0,0,$ $1,0,0,-1,$	0,0,0,0,	0,0,0,0,	0,0,0,0,	$-1,0,0,1$ $\big)$
$\frac{3-\sqrt{29}}{2} \approx -1.193$	$\left(\frac{10}{3-\sqrt{29}}, \frac{10}{3-\sqrt{29}}, \frac{10}{3-\sqrt{29}}, \frac{10}{3-\sqrt{29}}, \right.$ 1,1,1,1,	1,1,1,1,	1,1,1,1,	1,1,1,1,	1,1,1,1 $\big)$
$\frac{-1-\sqrt{21}}{2} \approx -2.791$	$\left(\frac{10}{-1-\sqrt{21}}, \frac{-10}{-1-\sqrt{21}}, 0,0, \right.$ $1,-1,0,0,$	$1,-1,0,0,$	$1,-1,0,0,$	$1,-1,0,0,$	$1,-1,0,0$ $\big)$
$\frac{-1-\sqrt{21}}{2} \approx -2.791$	$\left(\frac{10}{-1-\sqrt{21}}, 0, \frac{-10}{-1-\sqrt{21}}, 0, \right.$ $1,0,-1,0,$	$1,0,-1,0,$	$1,0,-1,0,$	$1,0,-1,0,$	$1,0,-1,0$ $\big)$
$\frac{-1-\sqrt{21}}{2} \approx -2.791$	$\left(\frac{10}{-1-\sqrt{21}}, 0,0, \frac{-10}{-1-\sqrt{21}}, \right.$ $1,0,0,-1,$	$1,0,0,-1,$	$1,0,0,-1,$	$1,0,0,-1,$	$1,0,0,-1$ $\big)$

Table 1: The eigenvalues and the corresponding eigenvectors of the adjacency matrix of the graph H_4.

there exists $\varepsilon > 0$ such that $f_1(\beta) > f_2(\beta)$ for all $\beta \in (0, \varepsilon)$. On the other hand, it holds that $f_1(1) < f_2(1)$; a direct computation shows that $f_1(1) \approx 6.481$ and $f_2(1) \approx 7.175$. Since both $f_1(\beta)$ and $f_2(\beta)$ are continuous functions of β on the interval $[0, 1]$, there exists $\beta \in (0, 1)$ such that $f_1(\beta) = f_2(\beta)$, i.e., such that all the diagonal entries of $e^{\beta \boldsymbol{A}}$ are the same. $\qquad\blacksquare$

A numerical computation yields that the value of β from the proof of Theorem 2 is approximately 0.499. There also exists $\beta > 1$ such that $f_1(\beta) = f_2(\beta)$. Indeed, assume that λ_1 is the largest eigenvalue of the adjacency matrix of the graph H_4 and let $\mathbf{u}_1$ be the corresponding unit eigenvector. Since $\mathbf{u}_{1,1}^2 > \mathbf{u}_{1,5}^2$, it follows from (1) that there exists $\beta_0 > 0$ such that $f_1(\beta) > f_2(\beta)$ for all $\beta \geq \beta_0$. Since $f_1(1) < f_2(1)$, we get that there exists $\beta \in (1, \beta_0)$ such that $f_1(\beta) = f_2(\beta)$; a numerical computation shows that the value of such β is approximately 1.912. We remark that each of the graphs H_m with $m \in \mathbb{N}$ greater than 1, has six different eigenvalues with the structure of corresponding eigenvectors similar to that of H_4.

We would like to conclude with an intuitive explanation behind the construction of the graph H_m. The graph H_m has vertices of degree m and $m + 1$, and any pair of vertices of the same degree can be mapped to each other by an automorphism of H_m. The values of the diagonal entries of $e^{\beta \boldsymbol{A}}$ are controlled by the diagonal entries of $\boldsymbol{A}^2$ for β close to zero, by the diagonal entries of $\boldsymbol{A}^3$ for larger (but still small) values of β, then by the diagonal entries of $\boldsymbol{A}^4$, etc. As k grows, the diagonal of $\boldsymbol{A}^k$ becomes proportional to the Perron-Frobenius eigenvector of $\boldsymbol{A}$. Hence, the diagonal entries of $e^{\beta \boldsymbol{A}}$ are proportional to the degrees of the corresponding vertices for the first regime of β, and to the eigenvector centrality of the vertices for β in the third regime (for a precise analysis, see [2]). In the graph H_m, the vertex degrees and Perron-Frobenius eigenvector values produce the same ordering on the vertices. On the other hand, the diagonal entries of $e^{\beta \boldsymbol{A}}$ corresponding to the vertices of degree m become larger than those corresponding to the vertices of degree $m + 1$ in the middle regime of β, since the vertices of degree m are contained in many triangles and cycles of length four. This explains the behavior of the functions f_1 and f_2 that we have observed in the proof of Theorem 2.

3 Temperatures classifying walk-regularity

We start by observing that a graph G achieves the maximum walk entropy for at most finitely many temperatures unless G is walk-regular.

Theorem 3. *If a graph G is not walk-regular, then there are only finitely many $\beta > 0$ such that $S^V(G, \beta) = \log n_G$.*

Proof. We proceed by contradiction. Suppose that there exists a graph G that is not walk-regular but the set I of $\beta \geq 0$ such that $S^V(G, \beta) = \log n_G$ is infinite.

Since the diagonal entries of $e^{\beta \boldsymbol{A}}$ are continuous functions of β bounded away from zero, it follows that $S^V(G, \beta)$ is continuous and the set I is closed. Let $\boldsymbol{A}$ be the adjacency matrix of G, $\lambda_1, \ldots, \lambda_k$ all distinct eigenvalues of $\boldsymbol{A}$, and $f_i(\beta)$ the i-th diagonal entry of $e^{\beta \boldsymbol{A}}$, $i = 1, \ldots, n_G$. We can assume that $\lambda_1 > \cdots > \lambda_k$. By (1), there exist non-negative reals a_{ij}, $i = 1, \ldots, n_G$ and $j = 1, \ldots, k$ such that

$$f_i(\beta) = \sum_{j=1}^{k} a_{ij} \cdot e^{\beta \lambda_j} \tag{2}$$

for every $i = 1, \ldots, n_G$ and $\beta \geq 0$. If $f_1(\beta) = \cdots = f_{n_G}(\beta)$ for all $\beta > 0$, G would be walk-regular by Theorem 1. Hence, $f_i \neq f_{i'}$ for some $i \neq i'$. By symmetry, we can assume that $f_1 \neq f_2$.

Let j be the smallest integer such that $a_{1j} \neq a_{2j}$. We can assume by symmetry that $a_{1j} > a_{2j}$, which implies that

$$\lim_{\beta \to \infty} (f_1(\beta) - f_2(\beta)) = \infty \ .$$

It follows that there exists β_0 such that $f_1(\beta) \neq f_2(\beta)$ for all $\beta \geq \beta_0$, i.e., the set I is a subset of the interval $[0, \beta_0)$. Since the set I is infinite, it has an accumulation point, which implies that G is walk-regular by Theorem 1, contrary to our original assumption. $\quad\square$

The next corollary immediately follows from Theorem 3.

Corollary 4. *There exists $\beta_0 > 0$ such that the following holds: a graph G is walk-regular if and only if $S^V(G, \beta_0) = \log n_G$.*

Proof. Let X be the set of all $\beta > 0$ such that there exists a graph G that is not walk-regular and $S^V(G, \beta) = \log n_G$. Since there are only finitely many such β for each non–walk-regular graph G by Theorem 3, the set X is countable. Hence, there exists $\beta_0 \in (0, \infty) \setminus X$ and any such β_0 has the property claimed in the statement of the corollary. $\quad\square$

4 Concluding remarks

Corollary 4 shows that there are temperatures $\beta_0 > 0$ such that, for any graph G, the graph G is walk-regular if and only if its walk entropy for β_0 is $\log n_G$. Unfortunately, we were not able to explicitly find any such β_0, and so it remains an open problem to identify a value β_0 with this property. It could be the case that $\beta_0 = 1$ is such a value of interest, as conjectured by Estrada [4].

Conjecture 4 (Estrada [4], Conjecture 3). *A graph G is walk-regular if and only if $S^V(G, 1) = \log n_G$.*

It could even be the case that for every non–walk-regular G, the walk entropy $S^V(G, \beta)$ is not maximized at any positive, rational value β_0.

Conjecture 5. *A graph G is walk-regular if and only if there exists a rational $\beta > 0$ such that $S^V(G, \beta) = \log n_G$.*

Theorem 3 asserts that if a graph G is not walk-regular, then the set of temperatures β such that $S^V(G, \beta) = \log n_G$ is finite. We believe that it is possible to bound the size of this set in terms of the number of vertices of G as follows.

Conjecture 6. *If a graph G is not walk-regular, then there are at most $n_G - 1$ values $\beta > 0$ such that $S^V(G, \beta) = \log n_G$.*

Acknowledgments

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