Walk entropy and walk-regularity

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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 \( \ell \). 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.

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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 \textit{walk-regular} \cite{walk-regular} if every vertex of \( G \) is contained in the same number of closed walks of length \( \ell \) 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 \( A^\ell \) of the adjacency matrix \( A \) 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.

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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

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

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 $[e^{\beta A}]_{ii}$, 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 $\beta$ 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 $A$ its adjacency matrix. Further, let $\lambda_1, \ldots, \lambda_{n_G}$ be the eigenvalues of $A$ and $u_1, \ldots, u_{n_G}$ an orthonormal basis formed by the eigenvectors of $A$. It follows that

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

for every $i = 1, \ldots, n_G$. In particular, each diagonal entry of $e^{\beta A}$ is an analytic function of $\beta$, 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 $A$ be the adjacency matrix of the graph $H_4$. The matrix $A$ has six different eigenvalues, which are given with corresponding eigenvectors in Table I. Note that the vectors given in Table I 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 $e^{\beta A}$ are the same, which yields the statement of the theorem.

Let $f_1(\beta) = [e^{\beta A}]_{11}$ and $f_2(\beta) = [e^{\beta A}]_{55}$. Note that $[e^{\beta A}]_{ii} = f_1(\beta)$ for $i = 1, \ldots, 4$ and $[e^{\beta A}]_{ii} = f_2(\beta)$ 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 $A^k$. 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
Table 1: The eigenvalues and the corresponding eigenvectors of the adjacency matrix $A_{K_4}$.

| Eigenvalue | Eigenvector |
|------------|-------------|
| $\pm\frac{\sqrt{5}}{2} \approx 2.236$ | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ |
| $\pm 3$ | $\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$ |
| $\pm\frac{\sqrt{5} - 1}{2} \approx 0.618$ | $\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ |

Figure 1: The graph $H_4$ and its adjacency matrix $A_{H_4}$.
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 $\beta$ 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 $e^{\beta A}$ are the same.

A numerical computation yields that the value of $\beta$ 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 $\lambda_1$ is the largest eigenvalue of the adjacency matrix of the graph $H_4$ and let $u_1$ be the corresponding unit eigenvector. Since $u_2^1 > u_1^5$, 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 $\beta$ is approximately 1.912.

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 $e^{\beta A}$ are controlled by the diagonal entries of $A^2$ for $\beta$ close to zero, by the diagonal entries of $A^3$ for larger (but still small) values of $\beta$, and then by the diagonal entries of $A^4$, etc. As $k$ grows, the diagonal of $A^k$ becomes proportional to the Perron-Frobenius eigenvector of $A$. Hence, the diagonal entries of $e^{\beta A}$ are proportional to the degrees of the corresponding vertices for the first regime of $\beta$, and to the eigenvector centrality of the vertices for $\beta$ 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 $e^{\beta A}$ corresponding to the vertices of degree $m$ become larger than those corresponding to the vertices of degree $m + 1$ in the middle regime of $\beta$, 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 $e^{\beta A}$ are continuous functions of $\beta$ bounded away from zero, it follows that $S^V(G, \beta)$ is continuous and the set $I$ is closed. Let $A$ be the adjacency matrix of $G$, $\lambda_1, \ldots, \lambda_k$ all distinct eigenvalues of $A$, and $f_i(\beta)$ the $i$-th diagonal entry of $e^{\beta A}$, $i = 1, \ldots, n_G$. 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

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

(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 $\beta_0$ 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.

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 $\beta$ 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 $\beta_0$ has the property claimed in the statement of the corollary.

## 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 $\beta_0$ is $\log n_G$. Unfortunately, we were not able to explicitly find any such $\beta_0$, and so it remains an open problem to identify a value $\beta_0$ 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 $\beta_0$.

**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 $\beta$ 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 $S^V(G, \beta) = \log n_G$.

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