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Maximum walk entropy implies walk regularity

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ABSTRACT

The notion of walk entropy $S^V(G,\beta)$ for a graph G at the inverse temperature β was put forward recently by Estrada et al. (2014) [7]. It was further proved by Benzi [1] that a graph is walk-regular if and only if its walk entropy is maximum for all temperatures $\beta \in I$, where I is a set of real numbers containing at least an accumulation point. Benzi [1] conjectured that walk regularity can be characterized by the walk entropy if and only if there is a $\beta > 0$ such that $S^V(G,\beta)$ is maximum. Here we prove that a graph is walk regular if and only if the $S^V(G,\beta = 1) = \ln n$. We also prove that if the graph is regular but not walk-regular $S^V(G,\beta) < \ln n$ for every $\beta > 0$ and $\lim_{\beta \to 0} S^V(G,\beta) = \ln n = \lim_{\beta \to \infty} S^V(G,\beta)$. If the graph is not regular then $S^V(G,\beta) \leq \ln n - \epsilon$ for every $\beta > 0$, for some $\epsilon > 0$.

1. Introduction

The concept of walk entropy was recently proposed as a way of characterizing graphs using statistical mechanics concepts [7]. For a simple, undirected graph $G = (V, E)$ with nodes $1 \leq i \leq n$ and adjacency matrix A the walk entropy is defined as

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

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where $p_i(\beta) = (e^{\beta A})_{ii}/Z$ and $\beta = 1/k_B T > 0$ (where k_B is the Boltzmann constant and T is the absolute temperature). Here $Z = \mathrm{tr}(e^{\beta A})$ represents the partition function of the graph, frequently referred to in the literature as the Estrada index of the graph [3,4,10]. The term $(e^{\beta A})_{ii}$ represents the weighted contribution of every subgraph to the centrality of the corresponding node, known as the subgraph centrality $SC(i)$ of the node [8,6,9]. The walk entropy called immediately the attention in the literature [1] due to its many interesting mathematical properties as well as its potential for characterizing graphs and networks. In [7] the authors stated a conjecture which was subsequently proved by Benzi [1] as the following

Theorem 1.1. *(See [1].) A graph G is walk-regular if and only if $S^V(G,\beta) = \ln n$ for all $\beta \geq 0$.*

Benzi [1] also reformulated another conjecture stated by Estrada et al. [7] in the following stronger form

Conjecture 1.2. *(See [1].) A graph is walk-regular if and only if there exists a $\beta > 0$ such that $S^V(G,\beta) = \ln n$.*

A third conjecture to be considered here generalizes the graphic examples given by Estrada et al. [7] and can be stated as

Conjecture 1.3. *Let G be a non-regular graph, then $S^V(G,\beta) < \ln n$ for every $\beta > 0$.*

In this note we prove these two conjectures, which immediately imply that the walk-entropy is a strong characterization of the walk-regularity in graphs and also gives strong mathematical support to the strength of this graph invariant for studying the structure of graphs and networks.

2. Main results

We start here by stating the two main results of this work.

Theorem 2.1. *Let A be the adjacency matrix of a connected graph G. Then the following conditions are equivalent:*

(a) *G is walk-regular;*
(b) *A^k has a constant diagonal for natural numbers k;*
(c) *e^A has constant diagonal;*
(d) *$e^{\beta A}$ has constant diagonal for $\beta \geq 0$;*
(e) *The walk entropy $S^V(G,1) = \ln n$.*

Theorem 2.2. *Let A be the adjacency matrix of a graph G. Then one and only one of the following conditions holds:*

(a) *G is walk-regular. Then $S^V(G,\beta) = \ln n$ for every $\beta > 0$;*
(b) *G is a regular but not walk-regular graph. Then $S^V(G,\beta) < \ln n$ for every $\beta > 0$. Moreover, $\lim_{\beta\to 0} S^V(G,\beta) = \ln n = \lim_{\beta\to\infty} S^V(G,\beta)$;*
(c) *There is some $\epsilon > 0$ such that $S^V(G,\beta) \leq \ln n - \epsilon$ for every $\beta > 0$.*

To avoid cross-reference in the proofs of the above theorems we present first the proof of Theorem 2.2.

3. Auxiliary definitions and results

Before stating the proof of Theorem 2.2 we need to introduce some definitions and auxiliary results, which are given below. We remind the reader that given a set $X = \{x_1, \dots, x_s\}$ of real numbers, the *variance* is defined as

$$\sigma^2(X) = E(X^2) - (E(X))^2 = \frac{1}{s}\sum_{i=1}^{s} x_i^2 - \left(\frac{1}{s}\sum_{i=1}^{s} x_i\right)^2.$$

Definition 3.1. Given a matrix M with diagonal entries $M_{11}, \dots, M_{nn}$, not all zero, we introduce the *diagonal variance* as

$$\sigma_d^2(M) = \frac{1}{\sum_{i=1}^{n} |M_{ii}|}\sigma^2(M_{11}, \dots, M_{nn}).$$

Let us now state and proof the following auxiliary result. We notice in passing that the diagonal variance of e^A was studied by Ejov et al. [5] in a different context for regular graphs.

Proposition 3.2. *Let A be the adjacency matrix of a connected graph G. Then one of the following conditions holds:*

(a) *e^A has constant diagonal;*
(b) *e^A has no constant diagonal entries and G is a regular graph. Then $\sigma_d^2(e^{\beta A}) > 0$ for $\beta > 0$ and $\lim_{\beta\to\infty} \sigma_d^2(e^{\beta A}) = 0$;*
(c) *There is some $\epsilon > 0$ such that $\sigma_d^2(e^{\beta A}) > \epsilon$ for every $\beta > 0$.*

Proof. We distinguish the following mutually excluding cases:

(1) G is walk-regular which implies that e^A has constant diagonal.

(2) $e^{\beta A}$ does not have constant diagonal entries, for any $\beta > 0$. Then $\sigma_d^2(e^{\beta A}) > 0$ for $\beta > 0$.

Observe that for $\beta > 0$ we have $(e^{\beta A})_{ii} \sim \phi_1^2(i)e^{\beta\lambda_1}$ and $Z(\beta A) \sim e^{\beta\lambda_1}$, where ϕ_1 is the (Perron) eigenvector of A corresponding to the maximal eigenvalue λ_1. Here the symbol $\sim$ means that the quantities are asymptotically equal.

In that situation

$$\lim_{\beta\to\infty} \sigma_d^2\big(e^{\beta A}\big) = \frac{1}{Z(\beta)}\sigma_d^2\big(\big(e^{\beta A}\big)_{ii} : 1 \le i \le n\big) = \sigma_d^2\big(\phi_1^2(i) : 1 \le i \le n\big).$$

Therefore $\lim_{\beta\to\infty}(e^{\beta A}) = 0$ is equivalent to ϕ_1 being constant, or G being regular. If G is not regular then the analytic function $\sigma_d^2(e^{\beta A}) > 0$, for $\beta > 0$, and $\lim_{\beta\to\infty} \sigma_d^2(e^{\beta A}) > 0$. Clearly, there is some $\epsilon > 0$ such that $\sigma_d^2(e^{\beta A}) \ge \epsilon$, for every $\beta > 0$. □

We continue now with some other auxiliary results needed to prove Theorem 2.2. Let $\lambda_1, \cdots, \lambda_n$ be the eigenvalues of A, such that $\sum_{j=1}^n \lambda_j = 0$ (since G is a simple graph without loops). For the vector of diagonal entries $y = (y_1, \cdots, y_n)$ of $e^{\beta A}$ we define a vector $z = \ln y = (\ln y_1, \cdots, \ln y_n)$ of real numbers. We have

$$\sum_{i=1}^n z_i e^{z_i} = \sum_{i=1}^n y_i \ln y_i$$

with $\sum_{i=1}^n z_i = \ln \prod_{i=1}^n y_i \ge \ln \det(e^{\beta A}) = \sum_{j=1}^n \lambda_j = 0$, where the inequality is a direct application of Hadamard's theorem for the positive definite matrix $e^{\beta A}$, see for instance [11]. The remarkable result of Borwein and Girgensohn [2] states the following.

Theorem 3.3. *Let $c_n = 2$ $(n = 2, 3, 4)$ and $c_n = e(1 - 1/n)$ $(n \ge 5)$. Let z_i be defined as before. Then [2] yields*

$$\frac{c_n}{n}\sum_{i=1}^n z_i^2 \le \sum_{i=1}^n z_i e^{z_i}.$$

4. Proof of Theorem 2.2

We know that $S^V(G, \beta) \le \ln n$ for every $\beta > 0$. Observe that for $Z(\beta) = \operatorname{tr}(e^{\beta A})$ the walk vertex entropy is

$$S^V(G, \beta) = \ln Z - \frac{1}{Z}\sum_{i=1}^n z_i e^{z_i}\Big|_\beta$$

The Borwein–Girgensohn inequality yields

$$S^V(G, \beta) \le \ln Z - \frac{1}{Z}\frac{c_n}{n}\sum_{i=1}^n z_i^2\Big|_\beta$$

We distinguish two situations at $\beta > 0$:

(1) $\sum_{i=1}^{n} z_i^2|_\beta = 0$, that is $y_i(\beta) = 1$ for $i = 1, \ldots, n$. Then, $Z(\beta) = n$ which is only possible if $A = 0$. Therefore $S^V(G, \gamma) = \ln n$ for any $\gamma > 0$.

(2) $\sum_{i=1}^{n} z_i^2 > 0$. Then there is a differentiable function $c_n \leq d_n(\beta)$ such that

$$S^V(G, \beta) = \ln Z - \frac{1}{Z} \frac{d_n}{n} \sum_{i=1}^{n} z_i^2 \Big|_\beta < \ln n.$$

Since $Z \geq n$ there is a differentiable function e_n satisfying $0 < e_n(\beta) \leq d_n(\beta)$ such that

$$S^V(G, \beta) = \ln n - \frac{e_n}{n^2} \sum_{i=1}^{n} z_i^2 \Big|_\beta.$$

For every $M > 0$, using the compactness of the interval $[0, M]$, there exists an $\epsilon(M) > 0$ such that $\frac{e_n}{n^2} \sum_{i=1}^{n} z_i^2|_\beta \geq \epsilon(M)$ for $\beta \in (0, M]$. Choose $\epsilon(M)$ such that

$$\inf\{\epsilon(M) : 0 < M\} = \lim_{\beta \to \infty} \frac{e_n}{n^2} \sum_{i=1}^{n} z_i^2 \Big|_\beta.$$

Moreover, recall from [7] that

$$S^V(G, \beta \to \infty) = -\sum_{i=1}^{n} \phi_1^2(i) \ln \phi_1^2(i).$$

This limit is $< \ln n$ except when there is a common value $\phi_1(i) = c_1$, for $i = 1, \ldots, n$. The latter property implies that G is a regular graph. We consider these cases separately.

(3) Assume that G is not a regular graph. Then $S^V(G, \beta \to \infty) < \ln n$. Therefore there exists an $\epsilon > 0$ such that for $M > 0$ we have $\epsilon(M) \geq \epsilon$. That is, $S^V(G, \beta) \leq \ln n - \epsilon$, for $\beta > 0$.

(4) Assume that G is a regular but not a walk-regular graph. Then, according with the analysis in Proposition 3.2, the maximal value $S^V(G, \beta) = \ln n$ is not attained for any $\beta > 0$. Moreover,

$$\lim_{\beta \to 0} S^V(G, \beta) = \ln n = \lim_{\beta \to \infty} S^V(G, \beta) \qquad \Box$$

5. Proof of Theorem 2.1

The following are obvious implications:

(a) implies (b), (a) implies (d), (d) implies (c), (c) implies (e), which leaves open only two implications.

For (b) implies (a), let

$$p(T) = T^n + p_{n-1} T^{n-1} + \cdots + p_0$$

be the characteristic polynomial of the graph G. The Cayley–Hamilton theorem yields $p(A) = 0$. If A^k has a constant diagonal for natural numbers $0 \le k \le m$ and $n - 1 \le m$, then

$$A^{m+1} = -\left(p_{n-1}A^m + \cdots + p_0 A^{m-n+1}\right)$$

has a constant diagonal.

(e) implies (a): follows from Theorem 2.2 □

In closing, the maximum of the walk entropy at $\beta = 1$, i.e., $S^V(G, 1) = \ln n$, is attained only for the walk-regular graphs. This means that $S^V(G, 1)$ can be used as an invariant to characterize walk-regularity in graphs.

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