

# 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  $\beta$  was put forward recently by Estrada et al. (2014) [6]. 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  $\beta \geq 0$ . Benzi (2014) [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  $\lim_{\beta \rightarrow 0} S^V(G, \beta) = \ln n = \lim_{\beta \rightarrow \infty} S^V(G, \beta)$ . If the graph is not regular then  $S^V(G, \beta) \leq \ln n - \varepsilon$  for every  $\beta > 0$  for some  $\varepsilon > 0$ .

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## 1. Introduction.

The concept of *walk entropy* was recently proposed as a way of characterizing graphs using statistical mechanics concepts [6]. For a simple, undirected graph  $G = (V, E)$  with  $n$  nodes  $1 \leq i \leq n$  and adjacency matrix  $A$  the walk entropy is defined as

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

where  $p_i(\beta) = \frac{[e^{\beta A}]_{ii}}{Z}$  and  $\beta = \frac{1}{k_B T} > 0$  ( $k_B$  is the Boltzmann constant and  $T$  the absolute temperature). Here  $Z = \text{Tr}[e^{\beta A}]$  represents the partition function of the graph, frequently referred in the literature as the Estrada index of the graph [3, 4, 9]. 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 [7, 5, 8]. The walk entropy called immediately the attention in the literature [1] due to its many interesting mathematical properties as well as its potentials for characterizing graphs and networks. In [6] the authors stated a conjecture which was subsequently proved by Benzi [1] as the following

**Theorem 1.1.** [1] A graph 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. [6] in the following stronger form

**Conjecture 1.2.** [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 was originally stated by Estrada et al. [6] as the following

**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  $0 \leq k \leq n-1$ ;
- (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 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,  $\lim_{\beta \rightarrow 0} S^V(G, \beta) = \ln n = \lim_{\beta \rightarrow \infty} S^V(G, \beta)$ ;
- (c) There is some  $\varepsilon > 0$  such that  $S^V(G, \beta) \leq \ln n - \varepsilon$  for every  $\beta > 0$ .

### 3. Proof of the Theorem 1

We start by seeing that (a) clearly implies (b). For (b) implies (a), let

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

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  $0 \leq k \leq m$  and  $n-1 \leq m$ , then

$$A^{m+1} = -(p_{n-1}A^m + \dots + p_0A^{m-n+1})$$

has a constant diagonal.

Clearly, (a) implies (d) which is equivalent to (c). We shall prove that (d) implies (b). We follow the techniques used for Theorem 2.1 in [1]. For  $1 \leq i \leq n$ , we consider

$$\varphi_0(\beta) \equiv \frac{1}{n} \text{Tr}(e^{\beta A}) = [e^{\beta A}]_{ii}$$

to be a real analytic function. As power series

$$\varphi_0(\beta) = 1 + \frac{\beta^2}{2!} k_i + \frac{\beta^3}{3!} [A^3]_{ii} + \frac{\beta^4}{4!} [A^4]_{ii} + \dots$$

using that  $G$  has no loops and  $[A^2]_{ii} = k_i$  is the degree of the node  $i$ . Consider the analytic function

$$\varphi_1(\beta) = \frac{2(\varphi_0(\beta) - 1)}{\beta^2} = k_i + \frac{\beta}{3} [A^3]_{ii} + \frac{\beta^2}{12} [A^4]_{ii} + \dots$$

and the limit  $k_i = \lim_{\beta \rightarrow 0} \varphi_1(\beta) = k$  is independent of the node, showing that  $G$  is regular.

Repeating the argument we get successively that  $[A^k]_{ii}$  is independent of the node  $i$  for  $k = 3, 4, \dots$ .

(d) implies (e): let  $y$  be the constant value of the entries of  $e^A$ . Then  $Z(1) = ny$  and

$$S^v(G, 1) = -n \left( \frac{y}{ny} \ln \frac{y}{ny} \right) = \ln n.$$

(e) implies (a): follows from Theorem 2.2. **Q.E.D.**

#### 4. Auxiliary definitions and results

Before stating the proof of the 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 4.1:** 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 prove the following auxiliary result.

**Proposition 4.2:** *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  $\lim_{\beta \rightarrow \infty} \sigma_d^2(e^{\beta A}) = 0$ ;
- (c) There is some  $\varepsilon > 0$  such that  $\sigma_d^2(e^{\beta A}) > \varepsilon$  for every  $\beta > 0$ .

**Proof:** We distinguish the following mutually excluding cases according to Theorem 1:

- (1)  $G$  is walk-regular, equivalently,  $e^A$  has constant diagonal.
- (2)  $e^{\beta A}$  has not constant diagonal, for any  $\beta > 0$ . Then  $\sigma_d^2(e^{\beta A}) > 0$  for  $\beta > 0$ .

Observe that for  $\beta \gg 0$  we have  $\lim_{\beta \rightarrow \infty} \left[ e^{\beta A} \right]_{ii} = \varphi_1^2(i) e^{\beta \lambda_1}$  and  $\lim_{\beta \rightarrow \infty} Z(\beta) = e^{\beta \lambda_1}$ , where  $\phi_1$  is the (Perron) eigenvector of  $A$  corresponding to the maximal eigenvalue  $\lambda_1$ . In that situation

$$\lim_{\beta \rightarrow \infty} \sigma_d^2(e^{\beta A}) = \frac{1}{Z(\beta)} \sigma_d^2\left(\left(e^{\beta A}\right)_{ii} : 1 \leq i \leq n\right) = \sigma_d^2\left(\varphi_1^2(i) : 1 \leq i \leq n\right).$$

Therefore  $\lim_{\beta \rightarrow \infty} \sigma_d^2(e^{\beta A}) = 0$  is equivalent to  $\phi_1$  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  $\lim_{\beta \rightarrow \infty} \sigma_d^2(e^{\beta A}) > 0$ . Clearly, there is some  $\varepsilon > 0$  such that  $\sigma_d^2(e^{\beta A}) \geq \varepsilon$  for every  $\beta > 0$ . **Q.E.D.**

We continue now with some other auxiliary results need to prove the Theorem 2. Let  $\lambda_1 > \lambda_2 \geq \dots \geq \lambda_n$  be the eigenvalues of  $A$ , such that  $\sum_{j=1}^n \lambda_j \geq 0$ . For the vector of diagonal entries  $y = (y_1, \dots, y_n)$  of  $e^{\beta A}$  we define a vector  $z = \ln y = (\ln y_1, \dots, \ln y_n)$  of real numbers. We have

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

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

**Theorem 4.3.** Let  $c_n = 2$  ( $n = 2, 3, 4$ ) and  $c_n = e(1 - 1/n)$  ( $n \geq 5$ ) and let  $z_i$  be defined as before. Then [2],

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

**Remarks 4.5.** (a) Observe that a priori it is not even clear that the sum  $\sum_{i=1}^n z_i e^{z_i}$  is positive. (b)

Borwein-Girgensohn inequality improves a previous bound given by Konstant and Michor [10].

## 5. Proof of the Theorem 2

We know that  $S^V(G, \beta) \leq \ln n$  for every  $\beta > 0$ . Observe that for  $Z(\beta) = \text{Tr}[e^{\beta A}]$  and the vertex entropy is

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

The Borwein-Girgerson [2] inequality yields

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

Moreover, the arithmetic mean-geometric mean inequality yields

$$Z(\beta) = \text{Tr}[e^{\beta A}] = \sum_{i=1}^n y_i \Big|_{\beta} \geq n \left( \prod_{i=1}^n e^{\lambda_i} \right) \Big|_{\beta}^{1/n} \geq n \left( e^{\beta \text{Tr}(A)} \right)^{1/n} \geq n$$

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

(1)  $\sum_{i=1}^n z_i^2 \Big|_{\beta} = 0$ , that is  $y_i(\beta) = 1$  for  $i = 1, \dots, n$ . Then,

$$Z(\beta) = \text{Tr}[e^{\beta A}] = \sum_{i=1}^n y_i(\beta) = n$$

and therefore

$$S^V(G, \beta) = \frac{n}{Z} \ln Z \Big|_{\beta} = \ln n.$$

In particular, for any  $\gamma > 0$ , the arithmetic-geometric mean inequality yields

$$n = Z(\gamma) = \text{Tr}[e^{\gamma A}] = \sum_{i=1}^n e^{\gamma \lambda_i} \geq n \left( \prod_{i=1}^n e^{\gamma \lambda_i} \right)^{1/n} = n \left( e^{\gamma \text{Tr}(A)} \right)^{1/n} = n$$

which implies that all  $e^{\gamma \lambda_i}$  have the same value, that is that all  $\gamma \lambda_i$  have the same value.

Since  $\text{Tr}[A] = 0$ , we have that  $\lambda_i = 0$  for  $i = 1, \dots, n$ . Then, the graph  $G$  is empty (it has no links) and  $S^V(G, \gamma) = \ln n$  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  $\varepsilon(M) > 0$  such that  $e_n(\beta) \geq \varepsilon_n(\beta)$  for  $\beta \in [0, M]$ . Moreover, recall from [3] that

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

This limit is  $< \ln n$  except when there is a common value  $\phi_1(i) = c_1$ ,  $i = 1, \dots, n$ . 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  $S^V(G, \beta \rightarrow \infty) < \ln n$ . Therefore there exists an

$\varepsilon > 0$  such that for  $\beta \in [0, \infty)$  we have

$$\frac{e_n}{n^2} \sum_{i=1}^n z_i^2 \Big|_{\beta} \geq \varepsilon.$$

that is,  $S^V(G, \beta) \leq \ln n - \varepsilon$ .

(4) Assume  $G$  is a regular graph. We may assume that  $G$  is not walk-regular. Then, according

with the analysis in [3], the maximal value  $S^V(G, \beta) = \ln n$  is not attained for any  $\beta$ . Moreover,

$$\lim_{\beta \rightarrow 0} S^V(G, \beta) = \ln n = \lim_{\beta \rightarrow \infty} S^V(G, \beta). \quad \mathbf{Q.E.D.}$$

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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