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A note on the entropy of graphs

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Abstract. A useful tool for investigation various problems in mathematical chemistry and computational physics is graph entropy. In this paper, we introduce a new version of graph entropy and then we determine it for some classes of graphs.

Keywords. graph eigenvalues, entropy, regular graph.

1 Introduction

Let G be a simple graph with adjacency matrix A. The Laplacian matrix of graph G is defined as $L = D - A$ where $D = [d_{ij}]$ is a diagonal matrix with $d_{ii} = deg_G(v_i)$, and $d_{ij} = 0$; otherwise. The spectra of L are a sequence of its eigenvalues displayed in increasing order, denoted by $LSepc(G) = \{0 = \mu_n, \mu_{n-1}, \ldots, \mu_1\}$. they are the roots of Laplacian characteristic polynomial $\phi_\mu(G) = det(\mu I - L)$. If G has exactly s distinct Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_s$ with multiplicity m_i, $(1 \leq i \leq s)$, then the Laplacian spectra of G is the following multiset [1]:

$$Lspec(G) = \{[\mu_1]^{m_1}, [\mu_2]^{m_2}, \ldots, [\mu_s]^{m_s}\}.$$

If we put $\gamma_i = \mu_i - \frac{2m}{n}$, then the Laplacian energy of G is defined as

$$LE(G) = \sum_{i=1}^{n} |\gamma_i|.$$

The graph entropy is a functional depending both on the graph itself and on a probability

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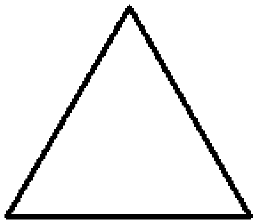

Figure 1. The cycle graph C_3.

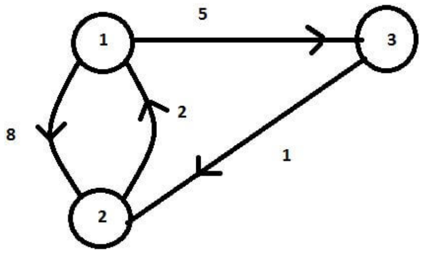

Figure 2. The directed cycle graph C_3.

distribution on its vertex set. This graph functional were proposed by a problem in information theory about source coding. It was introduced by J. Körner in 1973. Although the roots of graph entropy is in information theory, it was proved to be closely related to some classical and frequently studied graph theoretic concepts. von Neumann says the entropy of a system measures how much information the modelisation of a system does not provide.

To describe a vertex in a graph, we could use its degree, its eccentricity, its average distance from all vertices et cetera. But not necessarily these properties will describe that vertex. Consider, the cycle graph C_3 depicted in Figure 1. All vertices have the same properties. Their degree, their eccentricity, their average distance, etc are the same. Hence, it is impossible to provide enough information to identify it. In practice, this is a "high entropy" graph, because does not provide much information about its constituents. It is better to add at least a label to them, as the graph's topology does not help. Consider now the directed cycle graph C_3 in Figure 2. It is evident that there are no permutations which would leave the matrix unchanged and we can identify vertices related to entropy.

Suppose the logarithm based on 2 is denoted by the symbol log. Let $p = (p_1, \cdots, p_n)$ be a probability vector, namely $0 \leq p_i \leq 1$ and $\sum_{i=1}^{n} p_i = 1$. The Shannon's entropy [10] of p is defined as

$$I(p) = -\sum_{i=1}^{n} p_i log(p_i).$$

To define information-theoretic graph measures, we often consider a tuple $(\lambda_1, \cdots, \lambda_n)$ of non-negative integers $\lambda_i \in \mathbb{N}$. This tuple forms a probability distribution $p = (p_1, \cdots, p_n)$, see [2–9] where

$$p_i = \frac{\lambda_i}{\sum\limits_{j=1}^{n} \lambda_j}.$$

Therefore the entropy of tuple $(\lambda_1, \cdots, \lambda_n)$ is given by

$$I(\lambda_1, \cdots, \lambda_n) = -\sum_{i=1}^{n} p_i log(p_i) = log(\sum_{i=1}^{n} \lambda_i) - \sum_{i=1}^{n} \frac{\lambda_i}{\sum\limits_{j=1}^{n} \lambda_j} log(\lambda_i).$$

In the literature, there are various ways to obtain the tuple $(\lambda_1, \cdots, \lambda_n)$ like graph eigenvalues or partition-independent graph entropies, introduced by Dehmer [7] which are based on information functionals. Here, suppose $\mu_1, \cdots, \mu_n$ are Laplacian eigenvalues of G and $\gamma_i = \mu_i - \frac{2m}{n}$ $(1 \leq i \leq n)$, where $\gamma_i \neq 0$, then the entropy of G based on the Laplacian spectrum of G is defined as

$$I_L(G) = log(\sum_{i=1}^{n} |\gamma_i|) - \sum_{i=1}^{n} \frac{|\gamma_i|}{\sum\limits_{j=1}^{n} |\gamma_j|} log(|\gamma_i|) \tag{1}$$

$$= log(LE(G)) - \frac{1}{LE(G)} \sum_{i=1}^{n} |\gamma_i| log(|\gamma_i|). \tag{2}$$

Example 1.1. *The Laplacian eigenvalues of complete bipartite graph $K_{m,n}$ on $m+n$ vertices are*

$$[m+n]^1, [m]^{n-1}, [n]^{m-1}, [0]^1.$$

Hence,

$$LE(G) = \frac{2mn}{m+n} + \frac{2m}{n}$$

and thus

$$I_L(G) = log(\frac{2mn}{m+n} + \frac{2m}{n}) - \frac{1}{\frac{2mn}{m+n} + \frac{2m}{n}}(A),$$

where

$$A = \frac{m^2+n^2}{m+n} log(\frac{m^2+n^2}{m+n}) + \frac{m(n-1)(m-n)}{m+n} log(\frac{m(m-n)}{m+n})$$
$$+ \frac{n(m-1)(n-m)}{m+n} log(\frac{n(n-m)}{m+n}) + \frac{2m}{n} log(\frac{2m}{n}).$$

Theorem 1.2. *We have*

$$I_L(G) \geq log(\frac{LE(G)}{\Pi_{i=1}^{n} |\gamma_i|}).$$

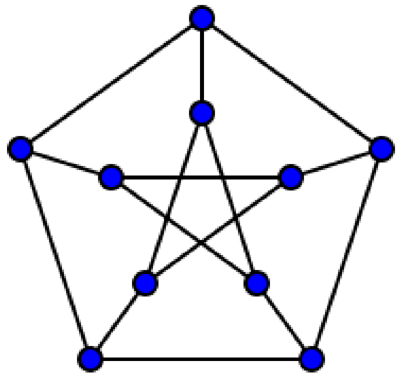

Figure 3. The Petersen graph P.

Proof. It is clear that

$$\sum_{i=1}^{n} |\gamma_i| log(|\gamma_i|) \leq \sum_{i=1}^{n} |\gamma_i| \sum_{i=1}^{n} log(|\gamma_i|).$$

This means that

$$I_L(G) \geq log(LE(G)) - \frac{LE(G)}{LE(G)} \sum_{i=1}^{n} log(|\gamma_i|) = log(LE(G)) - \sum_{i=1}^{n} log(|\gamma_i|).$$

Since $log(\frac{a}{b}) = log(a) - log(b)$, the proof is complete. □

Theorem 1.3. *Let G be a regular graph, then* $I_L(G) = I(G)$.

Proof. It is a well-known fact that if G is a k-regular graph with Laplacian eigenvalue μ corresponded to ordinary eigenvalue λ, then $\mu = k - \lambda$. This means that $|\gamma_i| = |\lambda_i|$ and the proof is complete. □

Example 1.4. *The Petersen graph P depicted in Figure 3 is an integral cubic graph with graph spectrum* $\{[-2]^4, [1]^5, [3]^1\}$. *Hence,* $LE(GP) = E(P) = 4.2 + 5.1 + 3.1 = 16$. *This means that*

$$I(P) = I_L(P) = log(16) - \frac{1}{16}\big(4 \times 2 \times log(2) + 3 \times log(3)\big) \approx 4.8.$$

Example 1.5. *The complete graph* K_n *is an integral* $(n-1)$*-regular graph with graph spectrum*

$$\{[-1]^{n-1}, [n-1]^1\}.$$

Hence,

$$I(P) = I_L(P) = log(2n-2) - \frac{n-1}{2n-2} log(n-1) = 1 + log(\sqrt{n-1}).$$

Example 1.6. *Consider the dodecahedron graph* C_{20} *depicted in Figure 4. This a cubic graph with graph spectrum*

$$\{[-\sqrt{5}]^6, [-2]^4, [0]^4, [1]^5, [3]^1\}.$$

Hence,

$$I(P) = I_L(P) \approx 3.$$

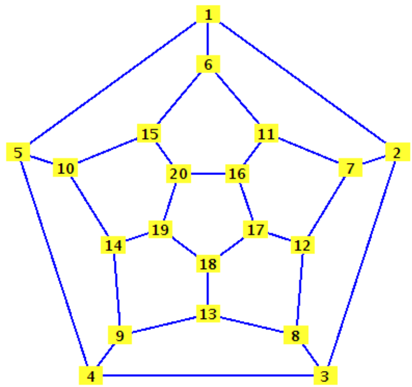

Figure 4. The dodecaheron C_{20}.

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