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Research article

Approximations for the von Neumann and Rényi entropies of graphs with circulant type Laplacians

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† We dedicate this paper to the memory of João da Providência, who unfortunately passed away just before the paper was published. da Providência played a crucial role in this research and he will be sorely missed.

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Abstract: In this note, we approximate the von Neumann and Rényi entropies of high-dimensional graphs using the Euler-Maclaurin summation formula. The obtained estimations have a considerable degree of accuracy. The performed experiments suggest some entropy problems concerning graphs whose Laplacians are g-circulant matrices, i.e., circulant matrices with g-periodic diagonals, or quasi-Toeplitz matrices. Quasi means that in a Toeplitz matrix the first two elements in the main diagonal, and the last two, differ from the remaining diagonal entries by a perturbation.

Keywords: entropy; graphs; Laplacian matrix; Euler-Maclaurin summation formula

1. Introduction

The notion of entropy is due to Rudolf Clausius (1850), and is linked with Carnot's famous theorem on the efficiency of thermal machines. This concept has many applications in different research areas, such as statistical mechanics, computation science, information theory, etc. The concept of graph entropy was introduced in information theory and is of special interest for understanding graph structure (see [1–8] and references therein).

Let G be an undirected graph with n vertices and at least one edge. The degree d_i of a vertex i is the number of edges incident on i. Let $L(G)$ be the Laplacian matrix of G, that is, $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix whose (i,i)-th entry is d_i and $A(G)$ is the (0,1) *adjacency matrix* of

G [9], i.e., a_{ij} is 1 if i, j are adjacent, and 0 otherwise. Since $L(G)$ is symmetric, its eigenvalues are real and as each row (and column) sum is 0, $L(G)$ is singular. Normalizing this matrix by its trace, we get the *density matrix of G,*

$$\rho_L(G) = \frac{1}{\mathrm{Tr}L(G)} L(G),$$

which is Hermitian with unit trace. By *Gershgorin Theorem*, all eigenvalues of $\rho_L(G)$ are nonnegative [10], so G can be seen as a quantum state. The eigenvalues of $\rho_L(G)$ constitute the *spectrum* of the graph G. In view of the above, it seems natural to investigate the information content of the graph as a quantum state [11].

For A and B positive semidefinite matrices such that $\mathrm{Tr}A = 1$, we consider the following matrix functions

$$S(A) = -\mathrm{Tr}(A \log A), \tag{1.1}$$

$$S(A, B) = \mathrm{Tr}A(\log A - \log B), \tag{1.2}$$

$$H_\alpha(A) = \frac{\log \mathrm{Tr}A^\alpha}{1-\alpha}, \quad \alpha \in (0,1) \cup (1,\infty), \tag{1.3}$$

$$H_\alpha(A, B) = \frac{\log \mathrm{Tr}A^\alpha B^{1-\alpha}}{\alpha - 1}, \quad \alpha \in (0,1) \cup (1,\infty). \tag{1.4}$$

The functions $S(A)$, $S(A, B)$, $H_\alpha(A)$ and $H_\alpha(A, B)$ are, respectively, the *von Neumann entropy* of A, the *von Neumann relative entropy* of A, B, the *α-Rényi entropy* of A and the *α-Rényi relative entropy* of A, B.

According to the *fundamental inequality of statistical thermodynamics* [12]

$$S(A, B) \geq \log \mathrm{Tr}B, \quad H_\alpha(A, B) \geq \log \mathrm{Tr}B.$$

For $\mathrm{Tr}B = 1$, we have $S(A, B) \geq 0$, and $H_\alpha(A, B) \geq 0$, with equality if $A = B$. So, $S(A, B)$ and $H_\alpha(A, B)$ may be conveniently used to measure the distance between the density matrices A and B. Obviously, $\lim_{\alpha\to 1} H_\alpha(A) = S(A)$ and $\lim_{\alpha\to 1} H_\alpha(A, B) = S(A, B)$.

Let G be a graph with at least one edge and let $\rho_1, \ldots, \rho_n$ be the eigenvalues of $\rho_L(G)$. We use the natural logarithm in the definitions of entropy and we make the convention that $0 \log 0 = 0$. The *von Neumann* entropy of the graph G, denoted $S_L(G)$, is the von Neumann entropy of $\rho_L(G)$. From (1.1),

$$S_L(G) := S(\rho_L(G)) = -\sum_{i=1}^{n} \rho_i \log \rho_i, \tag{1.5}$$

because $\rho_L(G)$ is unitarily diagonalizable and the logarithm is unitarily invariant. In terms of the eigenvalues $\lambda_1, \ldots, \lambda_n$ of the Laplacian $L(G)$, the von Neumann entropy of G is expressed as

$$S_L(G) = \log \sum_{k=1}^{n} \lambda_k - \left(\sum_{k=1}^{n} \lambda_k \right)^{-1} \sum_{k=1}^{n} \lambda_k \log \lambda_k. \tag{1.6}$$

The *α-Rényi entropy* of the graph G [13], denoted $H_\alpha(G)$, is the α-Rényi entropy of $\rho_L(G)$. For $\alpha \in (0,1) \cup (1,\infty)$ fixed, from (1.3) we have

$$H_\alpha(G) := H_\alpha(\rho_L(G)) = \frac{1}{1-\alpha} \log \sum_{i=1}^{n} \rho_i^\alpha. \tag{1.7}$$

In terms of the eigenvalues $\lambda_1, \ldots, \lambda_n$ of the Laplacian $L(G)$, the α-Rényi entropy of G is expressed as

$$H_\alpha(G) = \frac{1}{1-\alpha}\left(\log \sum_{k=1}^{n} \lambda_k^\alpha - \alpha \log \sum_{k=1}^{n} \lambda_k\right). \tag{1.8}$$

For a fixed graph G, the α-Rényi entropy $H_\alpha(G)$ is a monotonically decreasing function of α [2]:

$$H_\alpha(G) \leq H_{\alpha'}(G) \text{ for } \alpha > \alpha'.$$

The *complete graph* K_n is the one with the highest possible entropy. Indeed, if the density matrix ρ is singular, its highest possible entropy is $\log(n-1)$ and that is the entropy of the graph K_n. In terms of the eigenvalues λ_k and λ'_k, respectively of the Laplacian $L(G)$ and of the Laplacian $L(K_n)$, the *relative entropy* of G and K_n is given by

$$\begin{aligned} S(G, K_n) &:= S(\rho_L(G), \rho_L(K_n)) \\ &= \left(\sum_{j=1}^{n} \lambda_j\right)^{-1} \sum_{j=1}^{n} \lambda_j \left(\log \lambda_j - \log \lambda'_j\right) - \log \sum_{j=1}^{n} \lambda_j + \log \sum_{j=1}^{n} \lambda'_j, \end{aligned} \tag{1.9}$$

where λ_j and λ'_j are similarly, increasingly or decreasingly, ordered. Under these assumptions, the *α-relative Rényi entropy* of G and K_n is

$$\begin{aligned} H_\alpha(G, K_n) &:= H_\alpha(\rho_L(G), \rho_L(K_n)) \\ &= \frac{1}{\alpha - 1}\left(\log\left(\sum_{k=1}^{n} \lambda_k^\alpha {\lambda'}_k^{1-\alpha}\right) - \alpha \log \sum_{k=1}^{n} \lambda_k - (1-\alpha) \log \sum_{k=1}^{n} {\lambda'}_k\right). \end{aligned} \tag{1.10}$$

In recent years, many approaches to increase the understanding of graphical models have been developed, using entropic quantities associated to the graphs constructs (vertices, edges, etc), see e.g., Simmons et al. [6, 7] and references therein. The von Neumann entropy of graphs plays a major role in this program, namely by considering the von Neumann Theil index and its generalization by the Rényi entropy. In this note, using the Euler-Maclaurin formula we approximate the von Neumann and Rényi entropies of graphs of high dimensions whose Laplacians are g-circulant matrices, that is, circulant matrices where each row is a right cyclic shift in g-places to the preceding row. In the six cases we have studied, we observe that the relative entropy of G and K_n does not depend on n, for n sufficiently large. We have approximated the distance of the graph G to the graph K_n because K_n is the graph with n vertices with the highest entropy. From our investigations, the following problems arise.

Problem 1. Does the above mentioned observation hold for a general graph with a g-circulant Laplacian?

Problem 2. According to our experiments, we conclude that, for a fixed number of vertices, when the average number of incident edges on each vertex increases, the von Neumann and the α-Rényi entropies increase. Does this behaviour hold in general? When the number of vertices n is fixed, the average number of incident edges on each vertex is $2m/n$, where m is the number of edges, and the Problem may be rephrased in terms of the edges.

Problem 3. Does the question formulated in Problem 1 have a positive answer for a graph G whose Laplacian is the *quasi* g-Toeplitz matrix (see Case 6 below), obtained by cutting appropriate edges in a graph G with a g-circulant Laplacian? By a g-Toeplitz matrix we mean a matrix obtained from a g-circulant one by replacing its entries in the upper right and lower left corners by zeros.

2. Graph entropy for graphs with g-circulant Laplacians

Throughout the article the following form of the Euler-Maclaurin (E-M) formula will be used. For a proof, see, e.g., [14–17].

Lemma 1. *Let n be a positive integer and let f be a continuous real function in* $[0,1]$ *of class* $C^3(0,1)$*, i.e. with continuous derivaties until order* 3*. Then*

$$\sum_{k=1}^{n} f(\frac{k}{n}) = n\int_0^1 f(x)\mathrm{d}x + \frac{1}{2}(f(1)-f(0)) + \frac{1}{12n}(f'(1)-f'(0)) + R_n, \tag{2.1}$$

with

$$R_n = \frac{1}{6n^2}\int_0^1 B_3(\{nx\})f'''(x)\mathrm{d}x, \tag{2.2}$$

$B_3(x) = x^3 - 3x^2/2 + x/2$ *the third Bernoulli polynomial and* $\{x\}$ *the fractional part of x.*

Case 1

The Laplacian matrix of the cycle (or circuit) C_n is the $n \times n$ circulant matrix

$$L(C_n) = \begin{bmatrix} 2 & -1 & 0 & \dots & -1 \\ -1 & 2 & -1 & \dots & 0 \\ 0 & -1 & 2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \dots & 2 \end{bmatrix},$$

whose eigenvalues are

$$\lambda_k = 2 - 2\cos(2\pi k/n), \quad k = 1, 2, \dots n.$$

Therefore, the eigenvalues of $\rho_L(C_n)$ are $\rho_k = \lambda_k/(2n)$.

Consider $f(x) := (2-2\cos(2\pi x))\log(2-2\cos(2\pi x))$. By the Euler-Maclaurin formula and having in mind (1.6), we find

$$S(C_n) = \log(2n) - \frac{1}{2}(2 + \frac{R_n}{n}) = \log n - 0.306853 + \dots.$$

because the command *Integrate* of *Mathematica* yields

$$\int_0^1 (2-2\cos(2\pi x))\log(2-2\cos(2\pi x))\mathrm{d}x = 2.$$

We compute an upper bound for $|R_n|/n$. For $f(x) = (2-2\cos(2\pi x))\log(2-2\cos(2\pi x))$ in (2.2) and using the command *NIntegrate* of *Mathematica*, we find

$$\int_0^1 |f'''(x)|\mathrm{d}x = 24935.8,$$

so that

$$\frac{|R_n|}{n} \leq \frac{1}{6n^3} \times 0.0481125 \times \int_0^1 |f'''(x)|\mathrm{d}x = \frac{1}{6n^3} \times 0.0481125 \times 24935.8 = \frac{199.954}{n^3}.$$

From (1.9), we obtain the relative entropy of C_n and K_n,

$$S(C_n, K_n) = -\log(2n) + 1 + \log(n-1) + \ldots = -\log 2 + 1 + \ldots = 0.306853 + \ldots.$$

As $S(K_n) = \log(n-1)$, we have

$$\lim_{n\to\infty} S(C_n, K_n) = \lim_{n\to\infty}(S(C_n) - S(K_n)).$$

We study the asymptotic behavior of the 1/2-Rényi entropy of C_n for large n. We use (1.8), and we introduce the function of the real variable k/n, $f(k/n) := \lambda_k = 2 - 2\cos(2\pi k/n)$, with n a positive integer. In the spirit of the Euler-Maclaurin formula, we replace the sum

$$\sum_{k=1}^{n} \lambda_k^{1/2},$$

by the integral

$$\int_0^n f(k/n)^{1/2}\mathrm{d}k = n\int_0^1 f(x)^{1/2}\mathrm{d}x = n\int_0^1 (2 - 2\cos(2\pi x))^{1/2}\mathrm{d}x = \frac{4n}{\pi},$$

which has been evaluated using the command *Integrate* of *Mathematica*. Obviously, $\sum_{k=1}^n \lambda_k = 2n$. So, we have for the 1/2-Rényi entropy,

$$\begin{aligned} H_{1/2}(C_n) &= 2\left(\log\sum_{k=1}^{n}(2 - 2\cos(2\pi k/n))^{1/2} - \frac{1}{2}\log(2n)\right) \\ &= 2\left(\log\left(n\left(\frac{4}{\pi} + \frac{R_n}{n}\right)\right) - \frac{1}{2}\log(2n)\right) \\ &= \log n - 0.210018 + \ldots. \end{aligned}$$

We compute an upper bound for $|R_n|/n$. Using the command *NIntegrate* of *Mathematica* we find

$$\int_0^1 |f'''(x)|\mathrm{d}x = 24935.8,$$

so that by (2.2)

$$\frac{|R_n|}{n} \leq \frac{1}{6n^4} \times 0.0481125 \times \int_0^1 |f'''(x)|\mathrm{d}x = \frac{1}{6n^4} \times 0.0481125 \times 24935.8 = \frac{199.954}{n^4}.$$

For the 1/2-Rényi relative entropy of C_n and K_n, using (1.10), we obtain

$$H_{1/2}(C_n, K_n) = -2\log\left(\frac{4n}{\pi}\sqrt{n} + \ldots\right) + \log 2n + \log n(n-1)$$

$$= -2\log\left(\frac{4}{\pi}\right) + \log 2 + \ldots \approx 0.210018.$$

The asymptotic behavior of the 2-Rényi entropy of C_n for large n follows in a similar way, using the Euler-Maclaurin formula. Indeed, we replace the sum

$$\sum_{k=1}^{n} \lambda_k^2,$$

by the integral

$$\int_0^n (k/n)^2 \mathrm{d}k = n\int_0^1 f^2(x)\mathrm{d}x = n\int_0^1 (2-2\cos(2\pi x))^2 \mathrm{d}x = 6n,$$

and by (1.8), we get

$$\begin{aligned} H_2(C_n) &= -\left(\log \sum_{k=1}^{n} (2-2\cos(2\pi k/n))^2 - 2\log(2n)\right) \\ &\approx \log n - 0.405465. \end{aligned}$$

Case 2

Next we consider the graph with n vertices of the type represented in Figure 1. Its Laplacian, in the general case of n vertices, is the circulant matrix

$$A_n = \begin{bmatrix} 4 & -1 & -1 & 0 & 0 & \ldots & 0 & -1 & -1 \\ -1 & 4 & -1 & -1 & 0 & \ldots & 0 & 0 & -1 \\ -1 & -1 & 4 & -1 & -1 & \ldots & 0 & 0 & 0 \\ 0 & -1 & -1 & 4 & -1 & \ldots & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & 4 & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -1 & 0 & 0 & 0 & 0 & \ldots & -1 & 4 & -1 \\ -1 & -1 & 0 & 0 & 0 & \ldots & -1 & -1 & 4 \end{bmatrix} \in \mathbb{R}^{n\times n},$$

whose eigenvalues are

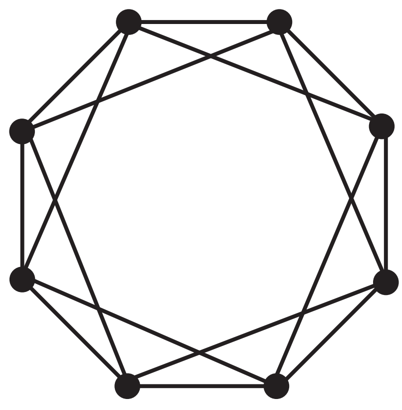

Figure 1

$$\lambda_k = 4 - 2\cos 2\pi k/n - 2\cos 4\pi k/n, \tag{2.3}$$

with $k = 1, \ldots, n$. The eigenvalues of the density matrix are $\rho_i = \lambda_i/(4n)$. Using the command *NIntegrate* of *Mathematica*, we find

$$\kappa := \int_0^1 (4 - 2\cos(2\pi x) - 2\cos(4\pi x))\log(4 - 2\cos(2\pi x) - 2\cos(4\pi x))\mathrm{d}x = 6.23166.$$

Using the Euler-Maclaurin formula, the von Neumann entropy of A_n is computed as

$$S(A_n) = \log(4n) - \frac{1}{4}(\kappa + \frac{R_n}{n}) = \log 4n - 1.55792 + \ldots \approx \log n - 0.171621. \tag{2.4}$$

An upper bound to $|R_n|/n$ is now estimated. Using the Command *NIntegrate* of *Mathematica* we find

$$\int |f'''(x)|\mathrm{d}x = 126619,$$

so that

$$\frac{|R_n|}{n} \leq \frac{302.593}{n^3}.$$

Notice that, for $f(x) = (4 - 2\cos(2\pi x) - 2\cos(4\pi x))\log(4 - 2\cos(2\pi x) - 2\cos(4\pi x))$, we have

$$f(0) - f(1) = f'(0) - f'(1) = 0.$$

In an analogous way, we also find

$$S(A_n, K_n) = 0.171621 + \ldots .$$

Since $S(K_n) = \log(n-1)$ and as the command *NIntegrate* of *Mathematica* yields

$$\int_0^1 (4 - 2\cos(2\pi x) - 2\cos(4\pi x))^{1/2}\mathrm{d}x = 1.88305,$$

we have

$$\lim_{n\to\infty} S(A_n, K_n) = \lim_{n\to\infty}(S(A_n) - S(K_n)).$$

In order to approximate the 1/2-Renyi entropy an analogous procedure holds. By (1.8) and as the command *NIntegrate* of *Mathematica* yields

$$\int_0^1 (4 - 2\cos(2\pi x) - 2\cos(4\pi x))^{1/2}\mathrm{d}x = 1.88305,$$

we obtain

$$H_{1/2}(A_n) = \log n + 2\left(\log(1.88305 + \frac{R_n}{n}) - \frac{1}{2}\log 4\right).$$

An upper bound to $|R_n|/n$ is estimated noticing that for $f(x) = (4 - 2\cos(2\pi x) - 2\cos(4\pi x))^{1/2}$, we have

$$f(0) - f(1) = f'(0) - f'(1) = 0.$$

Thus

$$H_{1/2}(A_n) \approx \log n - 0.12051.$$

From (1.10), we get

$$H_{1/2}(A_n, K_n) \approx 0.12051.$$

Case 3

The Laplacian of the graph with n vertices of the type represented in Figure 2 is

$$B_n = \begin{bmatrix} 6 & -1 & -1 & -1 & 0 & 0 & \dots & -1 & -1 & -1 \\ -1 & 6 & -1 & -1 & -1 & 0 & \dots & 0 & -1 & -1 \\ -1 & -1 & 6 & -1 & -1 & -1 & \dots & 0 & 0 & -1 \\ -1 & -1 & -1 & 6 & -1 & -1 & \dots & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & 6 & -1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -1 & -1 & 0 & 0 & 0 & 0 & \dots & -1 & 6 & -1 \\ -1 & -1 & -1 & 0 & 0 & 0 & \dots & -1 & -1 & 6 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

Its eigenvalues are

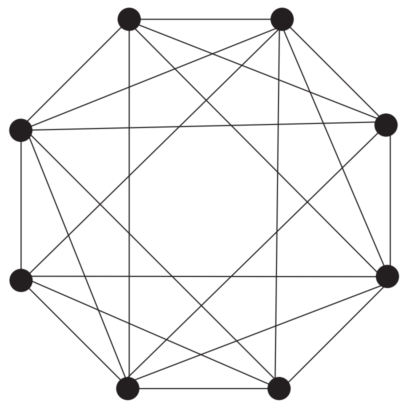

Figure 2

$$\lambda_k = 6 - 2\cos(2\pi k/n) - 2\cos(4\pi k/n) - 2\cos(6\pi k/n),$$

and the eigenvalues of the density matrix are $\rho_i = \lambda_i/(6n)$.

Using the Euler-Maclaurin formula, the von Neumann entropy is computed as

$$S(B_n) = -\sum_{k=1}^{n} \rho_i \log \rho_i = \log(6n) - \frac{1}{6}\kappa + \dots .$$

As by the command *NIntegrate* of *Mathematica*, we obtain

$$\kappa := \int_0^1 ((6 - 2\cos(2\pi x) - 2\cos(4\pi x) - 2\cos(6\pi x)) \\ \times \log(6 - 2\cos(2\pi x) - 2\cos(4\pi x)) - 2\cos(6\pi x))\mathrm{d}x = 11.4670,$$

we get

$$S(B_n) \approx \log n - 0.119406.$$

For the relative entropy, by (1.9), we obtain,

$$S(B_n, K_n) \approx 0.119406.$$

Using the Euler-MacLaurin formula, for $\rho(k) = \rho_k = \lambda_k / \sum_{j=1}^{n} \lambda_j$ and $f(n/k) = \lambda_k$, we have

$$\begin{aligned} H_\alpha(B_n) &= \frac{1}{1-\alpha}\left(\log\left(n\int_0^1 f^\alpha(x)\mathrm{d}x\right) - \alpha\log\sum_{k=1}^{n}\lambda_k + \ldots\right) \\ &= \frac{1}{1-\alpha}\left((1-\alpha)\log n + \log\int_0^1 f^\alpha(x)\mathrm{d}x - \alpha\log 6 + \ldots\right). \end{aligned}$$

Having in mind that

$$\kappa' := \int_0^1 (6 - 2\cos(2\pi x) - 2\cos(4\pi x) - 2\cos(6\pi x))^{1/2}\mathrm{d}x = 2.34793,$$

we get

$$H_{1/2}(B_n) \approx \log n + 2\log\kappa' - \log 6 = \log n - 0.0846939.$$

Case 4

The Laplacian of the graph with n vertices of the type represented in Figure 3 is the 2-circulant matrix

$$D_n = \begin{bmatrix} 4 & -1 & -1 & 0 & 0 & \ldots & 0 & -1 & -1 \\ -1 & 2 & -1 & 0 & 0 & \ldots & 0 & 0 & 0 \\ -1 & -1 & 4 & -1 & -1 & \ldots & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & \ldots & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & 4 & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -1 & 0 & 0 & 0 & 0 & \ldots & -1 & 4 & -1 \\ -1 & 0 & 0 & 0 & 0 & \ldots & 0 & -1 & 2 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

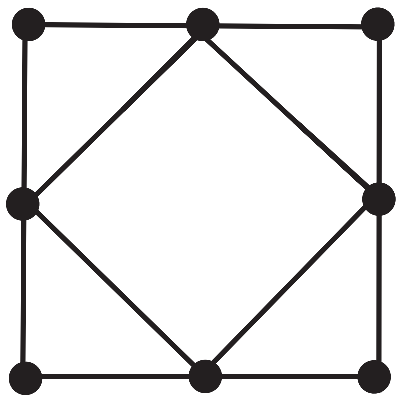

Figure 3

In order to determine the eigenvalues and eigenvectors of D_n we consider a vector of the form $w = (x\mathrm{e}^{i\theta_k}, y\mathrm{e}^{i\theta_k}, \ldots, x\mathrm{e}^{im\theta_k}, y\mathrm{e}^{im\theta_k})^\mathrm{T}$, $\theta_k = 2\pi k/m$, $k = 1, \ldots, m$, and the secular equation

$$D_n w = \lambda w,$$

which yields

$$\mathcal{S}(x,y)^{\mathrm{T}} = \lambda(x,y)^{\mathrm{T}},$$

where

$$\mathcal{S} = \begin{bmatrix} 4-2\cos\theta_k & -1-\mathrm{e}^{-i\theta_k} \\ -1-e^{i\theta_k} & 2 \end{bmatrix}, \quad \theta_k = \frac{2\pi k}{m}, \quad n = 2m, \ \ k = 1, \ \ldots, \ m,$$

The matrix $\mathcal{S}$ is called the symbol associated to D_n, and its eigenvalues are

$$\lambda_k^{(1,2)} = 3 - \cos\theta_k \pm \frac{\sqrt{7+\cos 2\theta_k}}{\sqrt{2}}.$$

Defining

$$\kappa_1 = \int_0^1 \left(3 - \cos 2\pi x - \sqrt{\frac{7+\cos 4\pi x}{2}}\right) \log\left(3 - \cos 2\pi x - \sqrt{\frac{7+\cos 4\pi x}{2}}\right) \mathrm{d}x,$$

$$\kappa_2 = \int_0^1 \left(3 - \cos 2\pi x + \sqrt{\frac{7+\cos 4\pi x}{2}}\right) \log\left(3 - \cos 2\pi x + \sqrt{\frac{7+\cos 4\pi x}{2}}\right) \mathrm{d}x,$$

we obtain, using the command *NIntegrate* of *Mathematica*,

$$\kappa_1 = 0.429296,$$

$$\kappa_2 = 7.75746,$$

and so

$$S(\rho(D_n)) = \log n - 0.265847 + \ldots\,.$$

For

$$\kappa_1' := \int_0^1 \left(3 - \cos 2\pi x + \sqrt{\frac{7+\cos 4\pi x}{2}}\right)^{1/2} \mathrm{d}x,$$

$$\kappa_2' := \int_0^1 \left(3 - \cos 2\pi x - \sqrt{\frac{7+\cos 4\pi x}{2}}\right)^{1/2} \mathrm{d}x,$$

we find, using the command *NIntegrate* of *Mathematica*,

$$\kappa_1' = 2.20059,$$

$$\kappa_2' = 0.973707,$$

and, using (1.8), we get

$$H_{1/2}(D_n) \approx \log n - 0.174734,$$

and

$$H_2(D_n) \approx \log n - 0.367725.$$

Case 5

The Laplacian of the graph with n vertices of the type represented in Figure 4, is the 3-circulant matrix

$$F_n = \begin{bmatrix} 4 & -1 & -1 & 0 & 0 & 0 & \dots & -1 & -1 \\ -1 & 3 & -1 & -1 & 0 & 0 & \dots & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & \dots & 0 & 0 \\ 0 & -1 & -1 & 4 & -1 & -1 & \dots & 0 & 0 \\ 0 & 0 & 0 & -1 & 3 & -1 & \dots & 0 & 0 \\ 0 & 0 & 0 & -1 & -1 & 3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & 0 & 0 & 0 & 0 & 0 & \dots & 3 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & \dots & -1 & 3 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

The symbol associated to F_n is

$$\mathcal{S} = \begin{bmatrix} 4 & -1-\mathrm{e}^{-i\theta_k} & -1-\mathrm{e}^{-i\theta_k} \\ -1-\mathrm{e}^{i\theta_k} & 3 & -1 \\ -1-\mathrm{e}^{i\theta_k} & -1 & 3 \end{bmatrix}, \quad \theta_k = \frac{2\pi k}{m}, \quad n = 3m,\ k = 1,\dots,m,$$

and its spectrum is

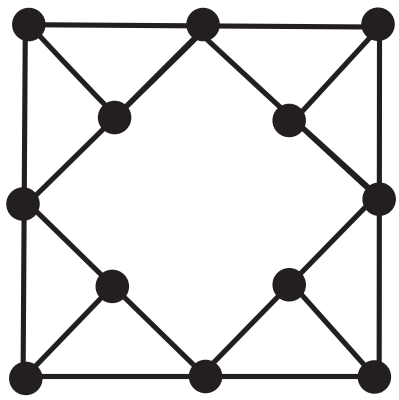

Figure 4

$$\sigma(\mathcal{S}) = \left\{4, 3 - \sqrt{4\cos\theta_k + 5}, 3 + \sqrt{4\cos\theta_k + 5}\right\}.$$

With the command *NIntegrate* of *Mathematica*, we find

$$\kappa_1 := \int_0^1 4\log 4\,\mathrm{d}x = 5.54518,$$

$$\kappa_2 := \int_0^1 \left(3 - \sqrt{4\cos\theta_k + 5}\right)\log\left(3 - \sqrt{4\cos\theta_k + 5}\right)\mathrm{d}x = 0.19892,$$

$$\kappa_3 := \int_0^1 \left(3 + \sqrt{4\cos\theta_k + 5}\right)\log\left(3 + \sqrt{4\cos\theta_k + 5}\right)\mathrm{d}x = 8.42759.$$

By (1.6), we get

$$S(F_n) = \log\frac{10n}{3} - \frac{1}{10}(\kappa_1 + \kappa_2 + \kappa_3) + \ldots = \log n - 0.213196 + \ldots .$$

Using the command *NIntegrate* of Mathematica, we find

$$\kappa_1' := \int_0^1 \sqrt{4}\,\mathrm{d}x = 2$$
$$\kappa_2' := \int_0^1 \left(3 - \sqrt{4\cos\theta_k + 5}\right)^{1/2}\,\mathrm{d}x = 0.973707,$$
$$\kappa_3' := \int_0^1 \left(3 + \sqrt{4\cos\theta_k + 5}\right)^{1/2}\,\mathrm{d}x = 2.20059.$$

Thus, by (1.8)

$$H_\alpha(F_n) = \log\frac{n}{3} + 2\log(\kappa_1' + \kappa_2' + \kappa_3') - \log 10 + \ldots \approx \log n - 0.148615.$$

Case 6

Up to now we have considered graphs with g-circulant Laplacians. Next, we evaluate the entropy of the graph of the type of the one in Figure 5, which is obtained by deleting in Figure 1 appropriate edges. Its Laplacian is the matrix

$$A_n' = \begin{bmatrix} 2 & -1 & -1 & 0 & \ldots & 0 & 0 & 0 \\ -1 & 3 & -1 & -1 & \ldots & 0 & 0 & 0 \\ -1 & -1 & 4 & -1 & \ldots & 0 & 0 & 0 \\ 0 & -1 & -1 & 4 & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & \ldots & -1 & -1 & 2 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

Let

$$A_n' = A_n + \Delta_n,$$

where

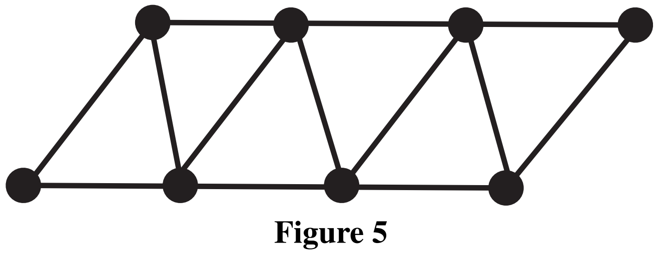

Figure 5

$$\Delta_n = -\begin{bmatrix} 2 & 0 & 0 & 0 & \dots & 0 & -1 & -1 \\ 0 & 1 & 0 & 0 & \dots & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & \dots & 0 & 1 & 0 \\ -1 & -1 & 0 & 0 & \dots & 0 & 0 & 2 \end{bmatrix} \in \mathbb{R}^{n\times n},$$

and let $A'_n(\eta) = A_n + \eta\Delta_n$. In the end we take $\eta = 1$. Regarding Δ_n as a perturbation of A_n, the eigenvalues of A'_n are easily obtained using perturbation theory. The eigenvalues of A_n are given by (2.3) and the respective eigenvectors are

$$u_k = \frac{1}{\sqrt{n}}(\mathrm{e}^{ik\theta_1}, \dots, \mathrm{e}^{ik\theta_n})^{\mathrm{T}}, \quad \theta_j = \frac{2\pi j}{n}, \quad j = 1, \dots, n.$$

We have, for the eigenvalues $\lambda_k(\eta)$ of $A'_n(\eta)$,

$$\lambda_k(\eta) = \lambda_k(0) + \eta\lambda'_k(0) + O(\eta^2).$$

See e.g., [18]. Then,

$$\delta\lambda_k = \lambda'_k(0) = u_k^*\Delta_n u_k = \frac{1}{n}(6 - 4\cos k\theta_{n-2} - 2\cos k\theta_{n-1}).$$

Theorem 2.1. *Under the above notations, we have*

$$\begin{aligned} &1) \quad \lim_{n\to\infty}(S(A'_n) - S(A_n)) = 0, \\ &2) \quad \lim_{n\to\infty}(S(A'_n, K_n) - S(A_n, K_n)) = 0, \\ &3) \quad \lim_{n\to\infty}(H_\alpha(A'_n) - H_\alpha(A_n)) = 0, \\ &4) \quad \lim_{n\to\infty}(H_\alpha(A'_n, K_n) - H_\alpha(A_n, K_n)) = 0. \end{aligned}$$

Proof. To approximate the entropy of A'_n we need the sum

$$\begin{aligned} &\sum_{j=1}^{n}(\lambda_k + \delta\lambda_k)\log(\lambda_k + \delta\lambda_k) = \sum_{j=1}^{n}(\lambda_k + \delta\lambda_k)\log(\lambda_k(1 + \delta\lambda_k/\lambda_k)) \\ &= \sum_{j=1}^{n}(\lambda_k + \delta\lambda_k)\left(\log\lambda_k + \frac{\delta\lambda_k}{\lambda_k} + \dots\right) \\ &= \sum_{j=1}^{n}\lambda_k\log\lambda_k + \sum_{j=1}^{n}\delta\lambda_k\,(1 + \log\lambda_k) + \dots, \end{aligned}$$

where we have neglected terms of higher order than the first, in the correction. We are therefore led, by the Euler-Maclaurin formula, to consider the integral

$$\int_0^1 (6 - 4\cos\frac{4\pi x}{n} - 2\cos\frac{2\pi x}{n})(1 + \log(4 - 2\cos 2\pi x - 2\cos 4\pi x))\mathrm{d}x.$$

For n large, we may replace this integral by

$$\frac{72}{n^2}\int_0^1 x^2(1+\log(4-2\cos 2\pi x-2\cos 4\pi x))\mathrm{d}x,$$

which is easily evaluated using *Mathematica*. If n is sufficiently large, the magnitude of the perturbation will be small enough in comparison with the magnitude of A_n and first order perturbation theory is valid. An approximation for $S(A'_n)$ will now be obtained:

$$\begin{aligned}
S(A'_n) &= \log\left(\sum_{k=1}^{n}(\lambda_k+\delta\lambda_k)\right) \\
&\quad -\left(\textstyle\sum_{k=1}^{n}(\lambda_k+\delta\lambda_k)\right)^{-1}\textstyle\sum_{k=1}^{n}(\lambda_k+\delta\lambda_k)\log(\lambda_k+\delta\lambda_k) \\
&= \log(4n-6)-\frac{1}{4n-6}\left(\sum_{k=1}^{n}\lambda_k\log\lambda_k+\sum_{k=1}^{n}\delta\lambda_k(1+\log\lambda_k)+\cdots\right) \\
&= \log(n-\frac{3}{2})+2\log 2-\frac{n\kappa}{4n-6} \\
&\quad -\frac{36}{n(2n-3)}\int_0^1 x^2(1+\log(4-2\cos 2\pi x-2\cos 4\pi x))\mathrm{d}x+\cdots \\
&= \log n+\log(1-\frac{3}{2n})+2\log 2-\frac{\kappa}{4}\cdot\frac{1}{1-\frac{3}{2n}} \\
&\quad -\frac{36}{n(2n-3)}\int_0^1 x^2(1+\log(4-2\cos 2\pi x-2\cos 4\pi x))\mathrm{d}x+\cdots \\
&= \log n-\frac{3}{2n}+\cdots+2\log 2-\frac{\kappa}{4}(1+\frac{3}{2n}+\cdots) \\
&\quad -\frac{36}{n(2n-3)}\int_0^1 x^2(1+\log(4-2\cos 2\pi x-2\cos 4\pi x))\mathrm{d}x+\cdots \\
&= S(A_n)-\frac{3}{2n}-\frac{3}{8n}\kappa \\
&\quad -\frac{36}{n(2n-3)}\int_0^1 x^2(1+\log(4-2\cos 2\pi x-2\cos 4\pi x))\mathrm{d}x+\cdots \\
&= \log n-0.171621-\frac{3.83687}{n}-\frac{10.5986}{n^2}+\ldots.
\end{aligned}$$

Hence, 1) follows. The remaining assertions are similarly shown.

3. Discussion

The obtained results for the first five cases previously considered, are summarized in Table 1. They lead to the conclusion that the relative entropy of the different graphs with respect to the complete graph K_n does not depend on n for sufficiently high n, and that the distance between the graphs G and K_n slightly decreases when the average number of incident edges on each vertex of G increases. We compute $H_2(G)$, the 2-Rényi entropy of G, by Eq (2) in [2], and then get the values of $\log_2 n - H_2(G)$. Compared with $H_2(G, K_n)$, the 2-relative Rényi entropy of G and K_n, our estimation method is better.

We have verified that $S(G, K_n)$ does not depend on n if n is large, and we have determined the $\lim_{n\to\infty} S(G, K_n)$, for several cyclic graphs G. We have seen that, asymptotically, $S(G, K_n)$ behaves like $S(K_n) - S(G)$. The following question naturally arises. Does $S(C_n, K_{1,n-1})$, where $K_{1,n-1}$ is the *star*

Table 1. Comparing relative von Neumann, 1/2-Rényi and the 2-Rényi entropies, for large n. In the last column the average number of incident edges in each vertex is shown.

G	$S(G, K_n)$	$H_{1/2}(G, K_n)$	$H_2(G, K_n)$	$\log_2 n - H_2(G)$	$\#d_{av}$
C_n	0.306853	0.210018	0.405465	0.584963	2
A_n	0.171621	0.120510	0.223144	0.321928	4
B_n	0.119406	0.0846939	0.154151	0.251062	6
D_n	0.265847	0.174734	0.367725	0.530515	3
F_n	0.213196	0.148615	0.277632	0.400538	10/3

graph, behave asymptotically like $S(K_{1,n-1}) - S(C_n)$? Let us compute $S(C_n, K_{1,n-1})$ using (1.6). The eigenvalues of $L(C_n)$ are $\lambda_k = 2 - 2\cos 2\pi k/n$, $k = 1, \ldots, n$, so, the highest eigenvalue of $L(C_n)$ is 2. The eigenvalues λ'_k of $L(K_{1,n-1})$ are 0, 1, with multiplicity $n-2$ and n. We find

$$\begin{aligned} & S(C_n, K_{1,n-1}) \\ &= \frac{1}{2n}\left(\sum_{k=1}^{n} \lambda_k \log \lambda_k - 2\log 2 + 2(\log 2 - \log n)\right) - \log 2n + \log 2(n-1) \\ &= 1 - \frac{\log n}{n} + \log(1 - 2/n) + \ldots, \end{aligned}$$

and so

$$\lim_{n\to\infty} S(C_n, K_{1,n-1}) = 1.$$

On the other hand

$$S(K_{1,n-1}) = -\frac{1}{2(n-1)} n \log n + \log 2(n-1),$$

and so

$$\lim_{n\to\infty} \frac{S(K_{1,n-1})}{\log n} = \frac{1}{2},$$

while

$$\lim_{n\to\infty} \frac{S(K_n)}{\log n} = \lim_{n\to\infty} \frac{S(C_n)}{\log n} = 1.$$

The answer to the above question is negative.

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Conflict of interest

The authors declare there is no conflicts of interest.

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