Note on von Neumann and Rényi entropies of a graph

Jephian C.-H. Lin

Department of Mathematics, Iowa State University

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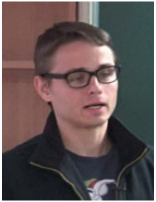
Joshua Lockhart

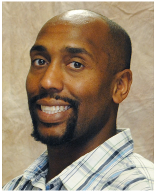
Michael Dairyko

Leslie Hogben



David Roberson

Simone Severini



Michael Young

Entropy

Let $\mathbf{p} = (p_1, p_2, \ldots, p_n)$ be a probability distribution, meaning

$$\sum_{i=1}^{n} p_i = 1 \text{ and } p_i \geq 0.$$

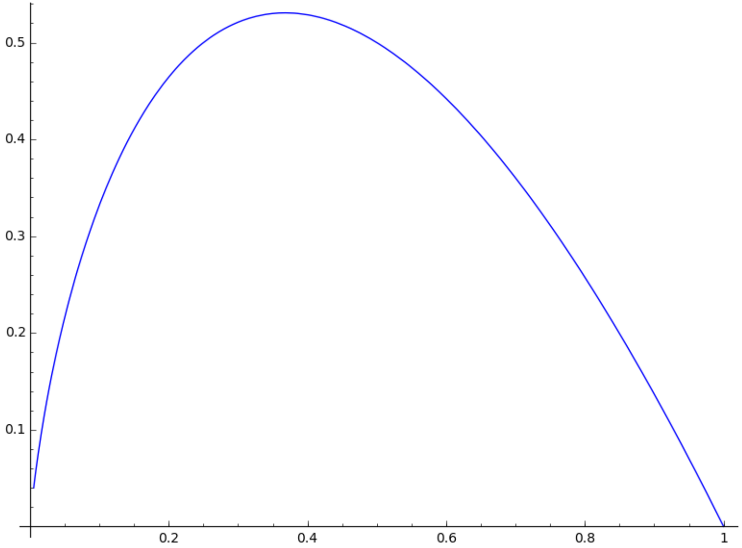
The Shannon entropy of $\mathbf{p}$ is

$$S(\mathbf{p}) = \sum_{i=1}^{n} p_i \log_2 \frac{1}{p_i}.$$

For a given $\alpha \geq 0$ with $\alpha \neq 1$, the Rényi entropy is

$$H_\alpha(\mathbf{p}) = \frac{1}{1-\alpha} \log_2 \left(\sum_{i=1}^{n} p_i^\alpha \right).$$

The function $x \log_2 \frac{1}{x}$



Convexity and Jensen's inequality

If f is a convex function, then Jensen's inequality says

$$\frac{1}{n}\sum f(p_i) \leq f\left(\frac{1}{n}\sum_{i=1}^{n} p_i\right).$$

Let $\overline{\mathbf{p}} = (\frac{1}{n}, \ldots, \frac{1}{n})$. Since $x \log_2 \frac{1}{x} \geq 0$ is convex,

$$0 \leq S(\mathbf{p}) \leq S(\overline{\mathbf{p}}) \text{ for all } \mathbf{p}.$$

Therefore, $S(\mathbf{p})$ is $\begin{cases} \text{maximized by } (\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}), \\ \text{minimized by } (1, 0, \ldots, 0). \end{cases}$

Entropy measures mixedness.

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Density matrix

A density matrix M is a (symmetric) positive semi-definite matrix with trace one. Every density matrix has the spectral decomposition

$$M = QDQ^\top = \sum_{i=1}^{n} \lambda_i \mathbf{v}_i \mathbf{v}_i^\top = \sum_{i=1}^{n} \lambda_i E_i,$$

where $\lambda_i \geq 0$ and $\sum_{i=1}^{n} \lambda_i = \mathrm{tr}(M) = 1$.

Each of E_i is of rank one and trace one; such a matrix is called a pure state in quantum information.

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Density matrix of a graph

Let G be a graph. The Laplacian matrix of G is a matrix L with

$$L_{i,j} = \begin{cases} d_i & \text{if } i = j, \\ -1 & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

Any Laplacian matrix is positive semi-definite and has

$$\mathrm{tr}(L) = \sum_{i=1}^{n} d_i = 2|E(G)| =: d_G.$$

The density matrix of G is $\rho(G) = \frac{1}{d_G} L$.

Entropies of a graph

Let G be a graph and $\rho(G)$ its density matrix. Then $\text{spec}(\rho(G))$ is a probability distribution.

The von Neumann entropy of a graph G is $S(G) = S(\text{spec}(\rho(G)))$; the Rényi entropy of a graph G is $H_\alpha(G) = H_\alpha(\text{spec}(\rho(G)))$.

Proposition

Let $G_1, \ldots, G_k$ be disjoint graphs, $c_i = \frac{d_{G_i}}{\sum_{i=1}^k d_{G_i}}$, and $\mathbf{c} = (c_1, \ldots, c_k)$. Then

$$S\left(\dot{\bigcup}_{i=1}^{k} G_i\right) = c_1 S(G_1) + \cdots + c_k S(G_k) + S(\mathbf{c}).$$

Union of graphs

Theorem (Passerini and Severini 2009)

If G_1 and G_2 are two graphs on the same vertex set and $E(G_1) \cap E(G_2) = \emptyset$, then

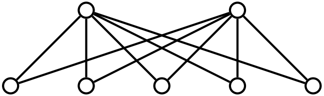
$$S(G_1 \cup G_2) \geq c_1 S(G_1) + c_2 S(G_2),$$

where $c_i = \frac{d_{G_i}}{d_{G_1} + d_{G_2}}$.

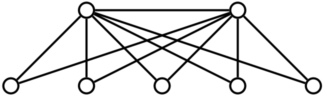
In particular, for a graph G and $e \in E(\overline{G})$, then

$$S(G + e) \geq \frac{d_G}{d_G + 2} S(G).$$

Adding an edge can decrease the von Neumann entropy



$K_{2,n-2}$



$K_{2,n-2} + e$

$$S(K_{2,n-2}) \sim 1 + (n-3) \cdot \frac{1}{2n-4} \log_2(2n-4)$$
$$S(K_{2,n-2} + e) \sim 1 + (n-3) \cdot \frac{1}{2n-3} \log_2(2n-3)$$

Extreme values of the von Neumann entropy

Recall $S(\mathbf{p})$ is $\begin{cases} \text{maximized by } (\frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n}), \\ \text{minimized by } (1, 0, \dots, 0). \end{cases}$

For graphs on n vertices, $S(G)$ is $\begin{cases} \text{maximized by } K_n, \\ \text{minimized by } K_2 \dot{\cup} (n-2)K_1. \end{cases}$

Conjecture (DHLLRSY 2017)

For connected graphs on n vertices, the minimum von Neumann entropy is attained by $K_{1,n-1}$.

Computational results and possible approaches

By Sage, $S(K_{1,n-1}) \leq S(G)$ for all connected graphs G on $n \leq 8$ vertices, and $S(K_{1,n-1}) \leq S(T)$ for all trees T on $n \leq 20$ vertices.

The conjecture is still open, but we can prove assymptotically.

Idea: The Rényi entropy $H_\alpha(\mathbf{p}) \nearrow S(\mathbf{p})$ as $\alpha \searrow 1$. In particular,

$$H_2(G) \leq S(G).$$

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What's nice about $H_2(G)$?

Let $M = \rho(G)$. Then by definition, the Rényi entropy $H_2(G)$ is

$$\frac{1}{1-2}\log_2\left(\sum_{i=1}^{n}\lambda_i^2\right) = -\log_2(\operatorname{tr} M^2) = \log_2\left(\frac{d_G^2}{d_G + \sum_i d_i^2}\right).$$

Theorem (DHLLRSY 2017)

If $\frac{d_G^2}{d_G + \sum_{i=1}^n d_i^2} \geq \frac{2n-2}{n^{\frac{n}{2n-2}}}$, *then* $S(G) \geq H_2(G) \geq S(K_{1,n-1})$.

It is known that $\sum_{i=1}^n d_i^2 \leq m\left(\frac{2m}{n-1} + n - 2\right)$. By some computation, almost all graphs have $S(G) \geq S(K_{1,n-1})$ when $n \to \infty$.

Conclusion

Whether $S(G) \geq S(K_{1,n-1})$ for all G or not remains open.

Conjecture (DHLLRSY 2017)

For every connected graph G on n vertices and $\alpha > 1$,

$$H_\alpha(G) \geq H_\alpha(K_{1,n-1}).$$

We are able to show $H_2(G) \geq H_2(K_{1,n-1})$ for every connected graphs on n vertices.

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