ENTROPY OF THE GIBBS STATE CANNOT DISTINGUISH COMPLEX GRAPH MODELS

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Abstract. In this work we study the entropy of the Gibbs state corresponding to a graph. The Gibbs state is obtained from the Laplacian, normalized Laplacian or adjacency matrices associated with a graph. We show that for a large number of graph models this approach does not distinguish the models asymptotically. We illustrate our analytical results with numerical simulations for Erdős-Rényi, Watts-Strogatz, Barabási-Albert and Chung-Lu graph models. We conclude saying that, from this perspective, these models are boring.

1. Introduction

A network represents a relationship among units of a complex system. The relations are encoded by edges while units are associated with nodes. Typical random graph models such as Erdős-Rényi graphs \cite{Erdos60} are usually not suitable for modeling real-world networks like the Internet \cite{Barabasi02}. Here complex network theory comes as a possible remedy. The boundary between a graph and a network is rather blurred, nevertheless a typical network is scale-free, small-world and has social structures. Typical examples of complex networks are Watts-Strogatz \cite{Watts98} and Barabási-Albert networks \cite{Barabasi99}.

Graph entropy describes the graph in the context of evolution on it \cite{Dorfman19}. In classical walks one typically considers the von Neumann entropy calculated for the Laplacian, as Laplacian defines valid continuous-time stochastic evolution \cite{vonNeumann27, alon2004}. Studies on various types of graph entropy can be found in the literature. The von Neumann entropy was first applied to complex networks in \cite{Kawashima08} and further developed in \cite{Dorfman19} and \cite{Dorfman19a}. Thermal state entanglement entropy on quantum graphs was studied in \cite{Glos08}. Entropy measure for complex networks using its Gibbs state was defined in \cite{Dorfman19}.

In contrary to stochastic evolution, continuous-time quantum walks accept arbitrary symmetric graph matrix which for undirected graphs includes adjacency matrix and normalized Laplacian \cite{Kawashima08, Glos12, Glos13}. Since it is known that the choice of a graph matrix does affect the evolution of quantum
walk \cite{11,12}, we claim that there is a need to design the entropy formula which accepts each of the above-mentioned matrices.

Entropy in the work \cite{4} is defined as the von Neumann entropy of Gibbs state of Laplacian matrix

\begin{equation}
S(\varrho_L) = -\text{Tr} \left( \frac{\exp(-\tau L)}{Z} \log \frac{\exp(-\tau L)}{Z} \right),
\end{equation}

where \(Z = \text{Tr} \exp(-\tau L)\) is a normalizing constant. Numerical calculations shed light on interesting behavior of the entropy depending on the parameter \(\tau\) of the Gibbs state interpreted as the inverse temperature or evolution time. However, the analysis made in \cite{4} was limited to fixed graph order \(n\). Nevertheless, it does not give a clue about the entropy’s behavior when one takes into consideration a fixed parameter \(\tau\) and varying graph order. Finally, while the entropy was originally defined for Laplacian, note that the Gibbs state is well-defined for an arbitrary Hamiltonian.

In this work we make the entropy analysis for other types of graph matrices, that is adjacency matrix and normalized Laplacian. On top of that we study the entropy of the Gibbs state with fixed parameter \(\tau\) for changing graph order \(n\). Numerical calculations for growing \(n\) reveal that the entropy is not able to detect the properties of complex networks. In other words, the entropy’s behavior does not change no matter which graph model is studied.

In \cite{4} authors point the phase transition of entropy value for Erdős-Rényi and Watts-Strogatz graphs for some critical value \(\tau_{\text{crit}}\). Our analytical considerations on Erdős-Rényi graphs confirm that such a phase transition actually occurs, however the value of \(\tau_{\text{crit}}\) depends on the graph order.

On top of that, we have calculated the entropy for some special graph classes for fixed parameter \(\tau\) and changing graph order \(n\). It appears that the entropy usually takes the form either \(o(1)\) or \(\log n - o(1)\), but nevertheless it is possible to find a counterexamples, which include complex networks.

This work is organized as follows. We begin with preliminaries in Section 2. Then, in Section 3 we present general theorems for entropy’s behavior basing on properties of the matrix spectra. The entropy values for specific graph classes are presented in Section 4 while the entropy’s behavior studied for various random graph models is described in Section 5. Eventually, conclusions can be found in Section 6.

2. Preliminaries

We will be interested in studying the von Neumann entropy of Gibbs states associated with a graph \(G\). A graph \(G\) is a pair \((V, E)\) where \(V\) is a set of vertices and \(E\) is a set of edges. In this work we restrict ourselves to simple undirected graphs. A graph has three typical matrix representations: the adjacency matrix, the Laplacian matrix and the normalized Laplacian matrix. The adjacency matrix of a simple graph is a symmetric square matrix consisting of ones if two vertices are adjacent and zeros otherwise. The adjacency matrix of a graph \(G\) will be denoted \(A(G)\). The degree matrix is a diagonal matrix with degrees of vertices on the diagonal. The degree matrix will be denoted \(D(G)\). We will often make use of (combinatorial) Laplacian matrix which is defined as \(L(G) := D(G) - A(G)\). The normalized Laplacian
is defined as $\mathcal{L}(G) := D(G)^{-\frac{1}{2}}L(G)D(G)^{-\frac{1}{2}} = I - D(G)^{-\frac{1}{2}}A(G)D(G)^{-\frac{1}{2}}$. When it will not make confusion we will be writing only $\mathcal{L}$ instead of $\mathcal{L}(G)$ and analogously for other graph matrices. Eigenvalues of matrices will be denoted $\lambda_1, \ldots, \lambda_n$, where $\lambda_1 \geq \cdots \geq \lambda_n$.

Now we will introduce the von Neumann entropy of a quantum state $\rho$. As $\rho$ is a density matrix, it is positive and has unit trace, its eigenvalues form a probability vector. Thus, the von Neumann entropy of the state $\rho$ is defined as the standard Shannon entropy of its eigenvalues. This fact can be succinctly written as

$$S(\rho) = -\text{Tr}(\rho \log(\rho))$$

where log refers to the natural logarithm throughout this paper.

For any Hermitian operator $H$ we can define an associated Gibbs state $\rho_H^\tau$ as

$$\rho_H^\tau = \frac{\exp(-\tau H)}{Z},$$

where $Z = \text{Tr}(\exp(-\tau H))$ is the partition function. The parameter $\tau$ can be regarded either as the inverse temperature or time [3]. Note that the von Neumann entropy of the Gibbs state can be written as [1]

$$S(\rho_H^\tau) = \tau \text{Tr}(H \rho_H^\tau) + \log Z.$$}

This entropy has two simple properties summarized in the following lemma, which proof is stated in the Appendix A.

**Lemma 1.** Let $H$ be a positive semidefinite matrix and $c \in \mathbb{R}$. It holds that $S(\rho_{cH}^\tau) = S(\rho_H^c \tau)$ and $S(\rho_{A+H}^\tau) = S(\rho_H^\tau)$.

We will be writing $S(\rho_H)$ instead of $S(\rho_H^\tau)$ when the value $\tau$ does not need to be stated explicitly.

When calculating the entropy of a graph given by the adjacency matrix we will use the notation $S(\rho_A)$ for $S(\rho_{A+H})$. When dealing with the Laplacian and normalized Laplacian matrices we will be writing $S(\rho_L)$ and $S(\rho_{L'})$ respectively.

### 3. General entropy properties

In this section we will present general theorems concerning the entropy’s behavior in which we assume only some restrictions on matrix spectra.

Let us begin with a proposition which shows a useful property of $d$-regular graphs. A $d$-regular graph is a graph whose all vertices have degree equal to $d$. For CTQW on $d$-regular graphs the evolution is independent on the choice of either adjacency matrix or Laplacian [6]. It follows from the fact that $D = dI$ and hence it affects only the global phase. For a similar reason, in the case of normalized Laplacian it can be seen as a change of time. It turns out that the proposed entropy reflects this behavior.

**Proposition 2.** Let $G$ be a $d$-regular graph. Then $S(\rho_A^\tau) = S(\rho_{L'}^\tau)$ and $S(\rho_L^\tau) = S(\rho_{A+H}^\tau/d)$.
Proof. Let $G$ be a $d$-regular graph. Then Laplace matrix of $G$ is $L = d1 - A$, where $A$ is the adjacency matrix of $G$. Now from Lemma 1 we have that $S(\varrho L) = S(\varrho^{-1}d - A) = S(\varrho^{-1}A)$.

The normalized Laplacian for the $d$-regular graph takes the form $L = 1 - \frac{1}{d}A$. Therefore again from Lemma 1 we have

$$S(\varrho L) = S(\varrho^{-1}d - A) = S(\varrho^{-1}A).$$

□

It turns out that for the normalized Laplacian the entropy may take the values only from the very small interval. Let us first present a result for general Hermitian matrices with bounded spectra. Its proof can be found in Appendix B.1

Lemma 3. Let $H$ be a matrix with eigenvalues bounded by $c_1 \geq \lambda_i \geq c_2$. Let $\tau > 0$ be a constant. Then

- if $c_1, c_2 \leq \frac{1}{\tau}$, then
  $$\log n - S(\varrho H) \leq \tau(c_1 - c_2),$$
- if $c_2 \leq \frac{1}{\tau} \leq c_1$, then
  $$\log n - S(\varrho H) \leq \tau(c_1 - \min\{c_1 \exp(\tau(c_2 - c_1)), c_2\}),$$
- if $c_1, c_2 \geq \frac{1}{\tau}$, then
  $$\log n - S(\varrho H) \leq \tau c_1(1 - \exp(\tau(c_2 - c_1))).$$

Conclusion directly drawn from the above Lemma is stated as a theorem concerning the entropy of a sequence of positive semidefinite matrices with finite spectral norm.

Theorem 4. Suppose $(H_n)$ is a sequence of positive semidefinite matrices $n \times n$ with spectral norm bounded by some constant independent of $n$. Then $S(\varrho H_n) = \log n - O(1)$.

For normalized Laplacian we have $c_2 = 0$ and $c_1 = \|L\| \leq 2 \|L\|$, which give us similar bounds as above. More specifically, independently on $\|L\|$ and $\tau$ the bound yields

$$\log n - S(\varrho H) \leq \tau \|L\|.$$ 

The bound cannot be improved to $\log n - o(1)$ for general normalized Laplacians sequence of growing size. In fact we will show, that the deviation from log($n$) occurs not only for simple graphs like cycle, but also for all complex graphs considered in this paper, see Sec. 5.

Note that for Laplacian matrices of graphs with maximal degree $\Delta$ we have $\Delta \leq \|L\| \leq 2\Delta$. Furthermore, for arbitrary graph we have $c_2 = 0$ for the Laplacian. Hence if a graph has a bounded degree, then we can simply utilize the Theorem 4 in this scenario.

While considering Laplacian matrices we need to assume that a matrix is singular. More specifically, the number of zero eigenvalues is equal to the number of connected components of the graph. We will focus on the case when one of the eigenvalues is equal to zero and the rest of the eigenvalues are strictly positive. In the next theorem we restrict ourselves to the case when all the nonzero eigenvalues converge to a positive constant.
Theorem 5. Let $H$ be a singular nonnegative matrix of size $n$ with single zero-eigenvalue and let $\tau > 0$ be a constant. Assume that $\lambda_1 \to c$ and $\lambda_{n-1} \to c$ for some constant $c$ as $n \to \infty$. Then $S(\varrho_H) = \log n - o(1)$.

The proof of the above theorem can be found in Appendix B.2.

Now we focus on the case when the spectrum can be unbounded. An example of such a matrix is a Laplacian matrix. While it is singular and positive semidefinite, its norm coincides with the maximum degree of the graph, hence it can be unbounded. In the following theorem, proven in Appendix B.3, we make an assumption only on the behavior of the smallest nonzero eigenvalue.

Theorem 6. Let $H_n$ be a singular nonnegative matrix of size $n$ with single zero-eigenvalue and let $\tau > 0$ be a constant. Assume $\lambda_{n-1}(H_n) \gg \log n$. Then $S(\varrho_{H_n}) = o(1)$.

We use the notation $f(x) \gg g(x)$ when $|f(x)/g(x)|$ goes to infinity as $x$ goes to infinity.

The Laplacian matrix of a connected graph does not necessarily satisfy the assumption on $\lambda_{n-1}$ mentioned in Theorem 6, hence the result cannot be generalized into ‘arbitrary sequence of Laplacians’, even connected. As an example, the cycle graph $C_n$ of size $n$ is known to have eigenvalues $2 - 2\cos\left(\frac{2\pi j}{n}\right)$ for $j = 0, \ldots, n - 1$. Hence the spectrum is bounded and we can apply Theorem 4. By this we have $S(\varrho_{L(C_n)}) = \log n - O(1)$. Such behavior shows the difference between Laplacian and normalized Laplacian in the sense of von Neumann entropy of the Gibbs state.

4. Entropy of specific graph classes

In this section we study the entropy of a few selected classes of graphs. The entropy is calculated for three types of graph matrices: adjacency matrix $A$, Laplacian matrix $L$ and normalized Laplacian $\mathcal{L}$. Four types of graphs were taken into consideration. An empty graph of order $n$ contains $n$ vertices and no edges. It is denoted by $E_n$. The symbol $K_n$ denotes the complete graph, that is the graph in which any two vertices are adjacent. A bipartite graph is a graph whose vertices are partitioned into two disjoint sets, $V$ and $W$, and any two vertices from the same set cannot be adjacent. When a vertex $v \in V$ is adjacent to all vertices from the set $W$ and vice-versa, then the graph is called a complete bipartite graph. Such a complete bipartite graphs where $|V| = n_1$ and $|W| = n_2$ is denoted by $K_{n_1,n_2}$. Finally, the symbol $C_n$ is used to denote a cycle graph.

All the results are presented in Table 1. The proofs can be found in Appendix C. An interesting observation is that in the first three cases the entropy behaves either like $\log n$ or converges to zero. For a cycle graph however the result is neither of them. More specifically, the entropy calculated for both adjacency and Laplacian matrices behaves in the same way

\begin{equation}
S(\varrho_{A(C_n)}) = S(\varrho_{L(C_n)}) = \log n - 2\tau \frac{I_1(2\tau)}{I_0(2\tau)} + \log (I_0(2\tau)) + o(1),
\end{equation}
Table 1. Asymptotic behavior of the entropy calculated for various graph classes described in Sec. 4

|       | adjacency matrix | Laplacian | normalized Laplacian |
|-------|------------------|-----------|----------------------|
| $E_n$ | $\log n - o(1)$ | $\log n - o(1)$ | $-$                  |
| $K_n$ | $o(1)$           | $o(1)$    | $\log n - o(1)$     |
| $K_{n_1, n_2}$ | $o(1)$   | depends on $n_1, n_2$ | $\log n - o(1)$ |
| $K_{n_1, n_1}$ | $o(1)$      | $o(1)$    | $\log n - o(1)$    |
| $C_n$ | $\log n - \Theta(1)$ | $\log n - \Theta(1)$ | $\log n - \Theta(1)$ |

where $I_\alpha(x)$ is the modified Bessel function of the first kind. For the normalized Laplacian of a cycle we obtain

$$S(\varrho L(C_n)) = \log n - \frac{I_1(\tau)}{I_0(\tau)} + \log (I_0(\tau)) + o(1).$$

It is also worth noting that the entropies calculated for adjacency matrix and Laplacian usually have the same asymptotic properties, that is either $\log n - o(1)$ or $o(1)$. Nevertheless, we found an counterexample which is a star graph $K_{n_1,1}$ for which the entropy for adjacency matrix is substantially different than the entropy for Laplacian.

5. Random graphs

In this section we consider various random graph models. Let us begin with Erdős-Rényi random graphs [1]. The symbol $G(n,p)$ is used to denote a random graph of order $n$ where the probability that any two vertices are adjacent equals $p$. A generalization of the Erdős-Rényi graph model is the Chung-Lu graph model [17,18] in which we obtain a graph with a specified expected degree sequence $(w_1, \ldots, w_n)$. The probability that vertices $v_i$ and $v_j$ are adjacent equals $w_i w_j / \sum_k w_k$.

Watts-Strogatz random graphs [3] are constructed as follows. In the first step we have a regular ring lattice, that is a graph of order $n$ where each vertex is adjacent to $K$ neighbors ($K/2$ on each side). Then for each vertex we consider their neighbors from one side and rewire them with probability $\beta$ to some other vertex. Watts-Strogatz graphs are known to be small-world, meaning that in contrary to Erdős-Rényi graphs all vertices are close to each other. Nevertheless, the degree distribution is highly concentrated around $K$.

Barabási-Albert random graphs [2] are constructed as follows. We begin with a complete graph with fixed order $m_0$. Then we add vertices one after another. Each time, a new vertex is adjacent to $m$ of the already existing vertices. The probability that the new vertex is adjacent to the already-existing vertex $v$ is proportional to the degree of the vertex $v$. We will start with analytical results for Erdős-Rényi and Chung-Lu graphs for Laplacian and normalized Laplacian matrices. Then, we will present
numerical results for other types of graph matrices and other graph models presented above.

5.1. **Erdős-Rényi graphs.** The Laplacian matrix of a random Erdős-Rényi graph with \( p \gg \log(n)/n \) almost surely has a single outlying zero eigenvalue and the rest of eigenvalues behaving like \( np(1 + o(1)) \). A useful property of the second smallest eigenvalue is formulated as a theorem.

**Theorem 7** (19). The second smallest eigenvalue \( \lambda_{n-1} \) of the random Laplacian matrix \( L \) from Erdős-Rényi graph \( G(n, p) \) with \( p \gg \log(n)/n \) satisfies a.a.s.

\[
\lambda_{n-1} = np + O(\sqrt{np\log n}).
\]

Moreover, from [12] we have that \( \lambda_1 \sim np \) for \( p \gg \log(n)/n \). The next remark follows from Theorem 6.

**Remark 8.** The von Neumann entropy of Gibbs state of Laplacian of random Erdős-Rényi graph \( G(n, p) \) with \( p \gg \log(n)/n \) converges a.a.s. to 0.

The main reason of such behavior is the strongly outlying 0 value. The behavior changes when \( p = \Theta(\log(n)/n) \). For \( p < (1 - \varepsilon)\log(n)/n \) the graph is almost surely disconnected [1], and since the dimensionality of the nullspace of the Laplacian equals the number of connected components [16], the graph entropy strongly depends on \( n \).

Let us now consider the threshold behavior of Erdős-Rényi model when \( p = p_0 \log n / n \) with \( p_0 > 1 \). Here we have \( \lambda_{n-1} \sim (1 - p_0)W_{-1}^{-1}\left(1 - p_0\right)e^{1-p_0}\log n \) [19] and \( \lambda_1 \sim (1 - p_0)W_{0}^{-1}\left(1 - p_0\right)e^{1-p_0}\log n \) [12], where \( W_{-1}, W_0 \) are Lambert \( W \) functions. In this case the following theorem provides results for selected values of \( \tau \). Its proof can be found in Appendix B.4.

**Theorem 9.** Let \( H_n \) be a positive semidefinite matrix with a single zero-eigenvalue of size \( n \) and \( \tau > 0 \) be a constant. Assume \( \lambda_{n-1} = a\log n \) and \( \lambda_1 = b\log n \) for \( a, b > 0 \). Then the behavior of the von Neumann entropy satisfies

1. if \( \tau < \frac{1}{b} \), then \( S(H_n) \geq (1 - \tau b)\log n + o(1) \),
2. if \( \tau = \frac{1}{b} \), then \( S(H_n) \geq \log 2 + o(1) \),
3. if \( \tau > \frac{1}{a} \), then \( S(H_n) = o(1) \).

For random Erdős-Rényi graphs the above theorem translates to the following remark.

**Remark 10.** Let \( H_n \) be a Laplacian matrix of a random Erdős-Rényi graph for \( p = p_0 \log n / n \) with \( p_0 > 1 \). Then

1. if \( \tau < W_{0}\left(1 - p_0\right)e^{1-p_0} \) / \((1 - p_0)\), then a.a.s. \( S(H_n) \geq C\log n + o(1) \) for some \( C \in (0, 1) \),
2. if \( \tau > W_{-1}\left(1 - p_0\right)e^{1-p_0} \) / \((1 - p_0)\), then a.a.s. \( S(H_n) = o(1) \).

Theorem 9 and Remarks 8, 10 give an analytical justification for the effect presented in [4]. The authors pointed that the phase-transition occurs with changing \( \tau \). This phase transition is shown in Figure 4 which shows
the value of the entropy of the Gibbs state for an Erdős-Rényi graph with
a function of the dimension of the graph and the parameter \( \tau \). We show
three values of the parameter \( p_0 \), namely \( p_0 = 10.5, 21, 42 \). To make it
easier to compare the values for changing dimensionality the value of the
entropy is normalized by dividing by \( \log n \). The phase transition is clearly
visible. We should also note that for sufficiently large dimension \( n \) the
normalized entropy does not depend on the dimension \( n \) around \( \tau < \frac{1}{b} \). Yet,
it still depends on \( \tau \) as stated by Theorem 9. A more detailed view on this
phenomenon is presented in Figure 4. It depicts this phase transition for the
ER, WS and BA models and for all considered graph matrices. The model
specific parameters are stated in the legend.

![Entropy of the Gibbs state as a function of the inverse temperature \( \tau \) and the dimension of the graph, \( n \) for the Erdős-Rényi model. The value of the entropy is normalized by dividing by \( \log n \). The phase transition can be easily seen. We show results for three values of the parameter \( p_0 \). The horizontal lines mark the theoretical boundaries for \( \tau \) found in Theorem 9 and Remark 10. The red line marks \( \tau = \frac{1}{b} \) while the white one corresponds to \( \tau = \frac{1}{a} \).](image)

Figure 1. Entropy of the Gibbs state as a function of the inverse temperature \( \tau \) and the dimension of the graph, \( n \) for the Erdős-Rényi model. The value of the entropy is normalized by dividing by \( \log n \). The phase transition can be easily seen. We show results for three values of the parameter \( p_0 \). The horizontal lines mark the theoretical boundaries for \( \tau \) found in Theorem 9 and Remark 10. The red line marks \( \tau = \frac{1}{b} \) while the white one corresponds to \( \tau = \frac{1}{a} \).

Theorem 9 not only confirms that there is a strong correlation between
spectral gap and the critical value of \( \tau \) but also shows that the transition
depends on the order of the graph \( n \). Further numerical investigation shows
that the entropy stabilizes with the graph order.

Let us now focus on the normalized Laplacian. It is known that normal-
ized Laplacian of random Erdős-Rényi graph satisfies requirements of
Theorem 9 for \( p \gg \log(n)/n \) [18], however, we can go beyond that. The
assumption can be relaxed to \( pn = (1 + \varepsilon) \log n \) for \( \varepsilon > 0 \) by Corollary 1.2
from [19]. We conclude our results with the following remark.
Remark 11. Assume \( L \) is a normalized Laplacian matrix of random Erdős–Rényi graph with \( p \geq (1 + \varepsilon) \log n/n \). The von Neumann entropy of Gibbs state \( \varrho_L \) satisfies a.a.s. \( \log n - o(1) \).

5.2. Chung-Lu graphs. By Theorem 4 from [18], normalized Laplacian of a random Chung-Lu graph for which minimum expected degree \( \omega_{\min} \gg \log n \) satisfies the requirement of Theorem 5. Therefore we have the following remark.

Remark 12. Assume \( L \) is a normalized Laplacian matrix of a Chung-Lu random graph for which minimum expected degree satisfies \( \omega_{\min} \gg \log n \). Then the von Neumann entropy of Gibbs state \( \varrho_L \) satisfies a.a.s. \( \log n - o(1) \).

The following remark concerns the case of adjacency matrix of a Chung-Lu random graph. Its proof can be found in Appendix B.5

Remark 13. Let \( A \) be an adjacency matrix of a random Chung-Lu graph with the maximum expected degree satisfying \( \omega_{\max} > \frac{6}{\eta} \log(\sqrt{2}n) \) and \( d := \frac{\sum \omega_i^2}{\sum \omega_i} \gg \omega_{\max} \sqrt{\log n} \). Then \( S(\varrho_A) = o(1) \).

5.3. Numerical insight. In this section we will complement the results concerning random graph models for all graph matrices presented in the preliminaries. In particular, we investigated the Watts-Strogatz model with parameters \( K = 4, \beta = 0.6 \), Barabási-Albert model with parameter \( m = 2 \) and Chung-Lu with expected degree sequence which mimic the Barabási-Albert model [20]. The inverse temperature is set to \( \tau = 0.1 \). All results are presented in Figure 2. As we can see almost all the graph models exhibit the same behavior.

On the other hand, for the rest of complex networks the plots are boring, which is compelling itself. This shows that the entropy of the Gibbs state lost the ability of recognizing properties distinguishing complex networks from nonphysical graphs when \( \tau \) is fixed. One could expect, that the deviation from \( \log(n) \) can serve as a method for recognizing these properties. However, on Figure 3 we can see that the deviations are of the same order. One could expect that for real-world networks, the deviation will be even more blurred, thus making it impossible to use it for recognizing properties of the models.

We claim, based on the results in [4], that this kind of information may be distilled from the localization and shape of the phase-transition. This is illustrated in Figure 4. While we can clearly observe the difference in shape between Erdős-Rényi graphs, Watts-Strogatz networks, and for Barabási-Albert with parameter \( m = 1 \). On the other hand for Barabási-Albert for \( m = 2, 3 \) we observe that the curve is similar as for Erdős-Rényi, the only difference is it in localization. Eventually, while there is a possibility to extract information about the graph from the phase transition, its detailed analysis may be too time-consuming to provide competitive method in network analysis.

All the code used to obtain the results presented here is available on GitHub at [https://github.com/iitis/graph-entropy](https://github.com/iitis/graph-entropy).
6. Conclusions

This work is focused on studying the entropy of the Gibbs state for various graphs. We made the analysis for three types of graph matrices: adjacency matrix, Laplacian and normalized Laplacian for various graph classes. It appeared that the asymptotic properties of the same graph may differ depending on which graph matrix is taken into consideration. Moreover, although the entropy usually takes the values either $\log n - o(1)$ or $o(1)$, for a cycle graph and complex networks the entropy value is none of them.

We considered also various random graph models. We studied analytically and numerically the entropy of Erdős-Rényi, Chung-Lu, Watts-Strogatz, Barabási-Albert random graphs for growing graph order and obtained that the entropy does not depend on which random graph model was studied when $\tau$ is fixed. Therefore one can draw a conclusion that the entropy is not able to detect the typical properties of complex networks like being small-world or scale-free. On the other hand, phase transition of the entropy in $\tau$ may posses such information.

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Figure 3. The value of $\log n - S(\rho_L)$ for the WS, BA and CL graphs plotted as function of the graph size $n$. Note that only in some cases this quantity vanishes for large $n$. The upper legend refers to the rewiring probability in the WS model. The bottom legend denotes the parameter $m$ for the BA model. The CL model was sampled in such a manner to produce expected degrees of vertices consistent with the BA model. Each line is obtained by averaging 100 randomly sampled graphs for each dimension $n$. The inverse temperature is $\tau = 0.1$.

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Figure 4. Illustration of the entropic phase transition for the ER, WS and BA models and all considered graph matrices. The value of the entropy is normalized by dividing by \( \log n \). The dimension is \( n = 200 \). The specific model parameters are stated in the corresponding legends. Each plot is obtained by averaging 100 randomly sampled graphs.

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Appendix A. Proof of properties of von Neumann entropy of the Gibbs state

Here we state the proof of claims made in Lemma 1.

Proof.

\begin{equation}
S(\varrho_{cH}) = \sum_{i=1}^{n} \lambda_i \exp \left( -\tau \lambda_i \right) + \log \left( \sum_{i=1}^{n} \exp \left( -\tau \lambda_i \right) \right).
\end{equation}

The numerator is a sum of eigenvalues mapped by \( f(x) = \tau x \exp (-\tau x) \) function. The function takes its unique maximum at \( x = 1/\tau \).

Let us begin with the case when \( c_1, c_2 \leq 1/\tau \). Then

\begin{equation}
S(\varrho_{cH}) \geq \frac{n \tau c_2 \exp (-\tau c_2)}{n \exp (-\tau c_2)} + \log (n \exp (-\tau c_1)) = \log n + \tau c_2 - \tau c_1,
\end{equation}

and therefore

\begin{equation}
\log n - S(\varrho_{cH}) \leq \tau (c_1 - c_2).
\end{equation}

If \( c_1, c_2 \geq 1/\tau \), then

\begin{equation}
S(\varrho_{cH}) \geq \frac{n \tau c_1 \exp (-\tau c_1)}{n \exp (-\tau c_2)} + \log (n \exp (-\tau c_1))
\end{equation}

\begin{equation}
= \tau c_1 (\exp (-\tau c_1 + \tau c_2)) + \log n - \tau c_1
\end{equation}

\begin{equation}
= \log n + \tau c_1 (\exp (\tau (c_2 - c_1)) - 1),
\end{equation}

\[ \square \]
Entropy of the Gibbs state cannot distinguish complex graph models

and hence

\[ \log n - S(\varrho_H) \leq \tau c_1 \left(1 - \exp \left(\tau (c_2 - c_1)\right)\right). \]

Assume finally that \( c_2 \leq \frac{1}{\tau} \leq c_1 \). In this case we have

\[ S(\varrho_H) \geq \frac{n \min \{c_1 \exp(-\tau c_1), c_2 \exp(-\tau c_2)\}}{n \exp(-\tau c_2)} + \log (n \exp(-\tau c_1)) \]

\[ = \tau \min \left\{ c_1 \exp(-\tau c_1), c_2 \exp(-\tau c_2) \right\} + \log n - \tau c_1 \]

\[ = \log n + \tau \left( \min \{c_1 \exp(\tau (c_2 - c_1)), c_2\} - c_1 \right), \]

and therefore

\[ \log n - S(\varrho_H) \leq \tau \left( c_1 - \min \{c_1 \exp(\tau (c_2 - c_1)), c_2\} \right). \]

\[ \Box \]

B.2. Proof of Theorem 5

Proof. The entropy takes the form

\[ S(\varrho_H) = \tau \text{Tr}(H \varrho_H^n) + \log Z \]

\[ = \tau \sum_{i=1}^{n} \lambda_i \exp(-\tau \lambda_i) + \log \left( \sum_{i=1}^{n} \exp(-\tau \lambda_i) \right). \]

Since the matrix \( H \) is singular, we can extract a single zero eigenvalue.

Hence the first part of the sum can be bounded as

\[ \tau (n-1) \lambda_{n-1} \exp(-\tau \lambda_{n-1}) \]

\[ \leq \tau \text{Tr}(H \varrho_H^n) \leq \frac{\tau (n-1) \lambda_1 \exp(-\tau \lambda_{n-1})}{1 + (n-1) \exp(-\tau \lambda_{n-1})} \]

Both bounds converge to \( \tau c \) and hence \( \tau \text{Tr}(H \varrho_H^n) \) as well converges to \( \tau c \).

Similarly for \( \log Z \) we have

\[ \log(1 + (n-1) \exp(-\tau \lambda_1)) \leq \log Z \leq \log(1 + (n-1) \exp(-\tau \lambda_{n-1})) \]

or equivalently

\[ \log \left( \frac{1}{n} + \frac{n-1}{n} \exp(-\tau \lambda_1) \right) \leq \log Z - \log n \leq \log \left( \frac{1}{n} + \frac{n-1}{n} \exp(-\tau \lambda_{n-1}) \right) \]

which implies \( \log Z - \log n \to -\tau c \) as \( n \to \infty \), which finishes the proof. \( \Box \)

B.3. Proof of Theorem 6

Proof. The entropy takes the form

\[ S(\varrho_{H_n}) = \tau \text{Tr}(H_n \varrho_{H_n}^n) + \log Z \]

\[ = \tau \sum_{i=1}^{n} \lambda_i \exp(-\tau \lambda_i) + \log \left( \sum_{i=1}^{n} \exp(-\tau \lambda_i) \right). \]

Since \( H_n \) matrix is singular, we can extract a single zero eigenvalue.
First we consider \( \tau \text{Tr}(H \varrho_{H_n}^\tau) \). Since \( x \exp(-x) \) is a decreasing function for \( x > 1 \) and since by assumption \( \tau \) is constant and \( \lambda_{n-1} \) tends to infinity, we can bound
\[
\tau \text{Tr}(H \varrho_{H_n}^\tau) \leq \frac{\tau(n-1)\lambda_{n-1} \exp(-\tau \lambda_{n-1})}{1 + (n-1) \exp(-\tau \lambda_1)} \\
\leq \tau(n-1)\lambda_{n-1} \exp(-\tau \lambda_{n-1}).
\]

Let \( \lambda_{n-1} = \log(n) g(n) \), where \( g(n) \gg 1 \). Then
\[
\tau(n-1)\lambda_{n-1} \exp(-\tau \lambda_{n-1}) = \tau(n-1) \log(n) g(n) n^{-\tau g(n)} \to 0 \quad \text{as} \quad n \to \infty.
\]

Now we bound
\[
\log Z \leq \sum_{i=1}^{n-1} \exp(-\tau \lambda_i) \leq (n-1) \exp(-\tau \lambda_{n-1}).
\]

If \( \lambda_{n-1} \gg \log n \), then the formula above tends to 0. Since both \( \tau \text{Tr}(H \varrho_{H_n}^\tau) \) and \( \log Z \) converge to zero we have the result. \( \square \)

B.4. Proof of Theorem 9

Proof. The entropy takes the form
\[
S(\varrho_{H_n}) = \tau \text{Tr}(H \varrho_{H_n}^\tau) + \log Z
\]
\[
= \frac{\tau}{\sum_{i=1}^{n} \lambda_i \exp(-\tau \lambda_i)} \sum_{i=1}^{n} \exp(-\tau \lambda_i) + \log \left( \sum_{i=1}^{n} \exp(-\tau \lambda_i) \right).
\]

Since the matrix \( H_n \) is singular, we can extract single zero eigenvalue.

The log \( Z \) part can be bounded as
\[
\log Z \leq \log(1 + (n-1) \exp(-\tau \lambda_{n-1}))
\]
\[
= \log(1 - n^{-\tau a} + n^{1-\tau a}),
\]
and
\[
\log Z \geq \log(1 + (n-1) \exp(-\tau \lambda_1))
\]
\[
= \log(1 - n^{-\tau b} + n^{1-\tau b}).
\]

Here behavior of \( \log Z \) depends on \( \tau \) parameter. If \( \tau < \frac{1}{b} \), then \( \log Z \geq (1-\tau b) \log n + o(1) \) and \( \log Z \leq (1-\tau a) \log n + o(1) \). If \( \tau > \frac{1}{a} \), then \( \log Z \) converges to 0.

In the \( \frac{1}{b} \leq \tau \leq \frac{1}{a} \) case we can provide partial results only. For \( \tau = \frac{1}{b} \) we have \( \log Z \geq \log 2 + o(1) \) and \( \log Z \leq (1-\frac{a}{b}) \log n + o(1) \). For \( \tau = \frac{1}{a} \) we have \( \log Z \leq \log 2 + o(1) \). For \( \tau \in (\frac{1}{b}, \frac{1}{a}) \) we can only provide \( \log Z \leq (1-\tau a) \log n + o(1) \).

Since \( H_n \) is a nonnegative matrix, we have \( \tau \text{Tr}(H_n \varrho_{H_n}^\tau) \geq 0 \). We can again provide simple bounds
\[
\tau \text{Tr}(H_n \varrho_{H_n}^\tau) \leq \frac{\tau(n-1)\lambda_{n-1} \exp(-\tau \lambda_{n-1})}{1 + (n-1) \exp(-\tau \lambda_1)} \\
\leq \frac{\tau(n-1) \lambda \log n \exp(-\tau a \log n)}{(n-1) \exp(-\tau b \log n)} \\
= \frac{\tau n^{\tau (b-a)}}{\log n},
\]
and similarly
\[
\tau \text{Tr}(H_n \varrho_{H_n}) \geq \frac{\tau (n-1) \lambda_1 \exp(-\tau \lambda_1)}{1 + (n-1) \exp(-\tau \lambda_{n-1})}
\geq \frac{\tau (n-1)b \log n \exp(-\tau b \log n)}{n \exp(-\tau a \log n)}
= \frac{n-1}{n} \tau b \log \frac{n}{\exp(-\tau a \log n)}.
\]

By combining the above inequalities we obtain the result. □

B.5. Proof of Remark 13

Proof. Let \( \lambda_n(-A) < 0 \) be the single outlying eigenvalue of the matrix \(-A\). By the use of Theorem 3 from [18] we have the bound
\[
|\lambda_i(A)| \leq \sqrt{8 \omega_{\text{max}} \log(\sqrt{2}n)}
\]
for \( i = 1, \ldots, n - 1 \). From Lemma 11 we note that
\[
S(\varrho_{A}) = S(\varrho_{-\lambda_n 1 + A})
\]
and therefore it suffices to consider the case of a shifted spectrum with single zero eigenvalue and where for all the other eigenvalues we have
\[
\lambda_i(-\lambda_n I + A) = \lambda_i(A) + \lambda_n(-A) \geq \tilde{d} - 2 \sqrt{8 \omega_{\text{max}} \log(\sqrt{2}n)}.
\]
Using the assumption on \( \tilde{d} \), asymptotically we obtain \( \lambda_i(-\lambda_n I + A) \gg \log n \) for \( i = 1, \ldots, n - 1 \). Then we use Theorem 9 □

APPENDIX C. Entropy of specific graph classes - proofs

The analytical spectra of all the graph classes discussed in this appendix are taken from [16].

C.1. Complete graph. The Laplacian matrix of the complete graph has a single eigenvalue equal to zero and \( n - 1 \) eigenvalues equal to \( n \). Therefore
\[
S(\varrho_{L(K_n)}) = \tau \sum_{i=1}^{n} \lambda_i \exp(-\tau \lambda_i) + \log \left( \sum_{i=1}^{n} \exp(-\tau \lambda_i) \right)
= n\tau \left( 1 - \frac{1}{1 + (n-1) \exp(-n\tau)} \right) + \log (1 + (n-1) \exp(-n\tau))
= o(1).
\]
As the complete graph is a regular graph, then from Proposition 2 we have \( S(\varrho_{L(K_n)}) = S(\varrho_{A(K_n)}) \). In the case of normalized Laplacian we use the fact that the complete graph is a \((n-1)\)-regular graph. Therefore the spectrum of the normalized Laplacian consists of \( n - 1 \) eigenvalues equal to \( \frac{n}{n-1} \) and
a single eigenvalue equal to 0. Therefore we calculate
\begin{equation}
\begin{aligned}
S(\theta_L(K_n)) &= \tau \frac{n \exp\left(-\tau \frac{n}{n-1}\right)}{1 + (n-1) \exp\left(-\tau \frac{n}{n-1}\right)} + \log \left(1 + (n-1) \exp\left(-\tau \frac{n}{n-1}\right)\right) \\
&= \log n - o(1).
\end{aligned}
\end{equation}

C.2. Complete bipartite graph. Now we study entropy of the complete bipartite graph. Let us set $|V| = n_1$ and $|W| = n_2$. The spectrum of the adjacency matrix of such a complete bipartite graph $K_{n_1,n_2}$ consists of $n_1 + n_2 - 2$ zero eigenvalues and $\pm \sqrt{n_1 n_2}$. Therefore we have
\begin{equation}
\begin{aligned}
S\left(\theta_A(K_{n_1,n_2})\right) &= \tau \sqrt{n_1 n_2} \left(1 - \frac{2 \exp(\tau \sqrt{n_1 n_2}) + n_1 + n_2 - 2}{\exp(-\tau \sqrt{n_1 n_2}) + \exp(\tau \sqrt{n_1 n_2}) + n_1 + n_2 - 2}\right) \\
&+ \tau \sqrt{n_1 n_2} + \log \left(1 + \exp(-2\tau \sqrt{n_1 n_2}) + \frac{n_1 + n_2 - 2}{\exp(\tau \sqrt{n_1 n_2})}\right) = o(1).
\end{aligned}
\end{equation}

The spectrum of the Laplacian of the complete bipartite graph consists of a single 0 eigenvalue, $n_1 - 1$ eigenvalues equal $n_2$, $n_2 - 1$ eigenvalues equal $n_1$, and a single $n_1 + n_2$ eigenvalue. Now we assume $n_1 = n_2$ and calculate
\begin{equation}
\begin{aligned}
S\left(\theta_L(K_{n_1,n_1})\right) &= \tau n_1 \left(1 - \frac{1 - \exp(-2\tau n_1)}{1 + 2(n_1 - 1) \exp(-\tau n_1) + \exp(-2\tau n_1)}\right) \\
&+ \log \left(1 + 2(n_1 - 1) \exp(-\tau n_1) + \exp(-2\tau n_1)\right) = o(1).
\end{aligned}
\end{equation}

Assuming $n_2 = 1$ we obtain
\begin{equation}
\begin{aligned}
S\left(\theta_L(K_{n_1,1})\right) &= \tau \left(1 - \frac{1 - n_1 \exp(-\tau (n_1 + 1))}{1 + (n_1 - 1) \exp(-\tau) + \exp(-\tau (n_1 + 1))}\right) \\
&+ \log \left(1 + n_1 \exp(-\tau) - \exp(-\tau) + \exp(-\tau (n_1 + 1))\right) \\
&= \log(n_1 + 1) - o(1).
\end{aligned}
\end{equation}

Eigenvalues of a normalized Laplacian of a $K_{n_1,n_1}$ graph consist of single eigenvalues equal 0 and 2, and $2n_1 - 2$ eigenvalues equal 1. Therefore
\begin{equation}
\begin{aligned}
S\left(\theta_L(K_{n_1,n_1})\right) &= \tau \left(1 - \frac{1 - \exp(-2\tau)}{1 + (2n_1 - 2) \exp(-\tau) + \exp(-2\tau)}\right) \\
&+ \log \left(1 + (2n_1 - 2) \exp(-\tau) + \exp(-2\tau)\right) \\
&= \log(2n_1) - o(1).
\end{aligned}
\end{equation}

Eigenvalues of a normalized Laplacian of a star graph $K_{n_1,1}$ consist of a single 0 eigenvalue, $n_1 - 1$ eigenvalues equal 1 and a single eigenvalue equal 2. Thus we have
\begin{equation}
\begin{aligned}
S\left(\theta_L(K_{n_1,1})\right) &= \tau \left(1 - \frac{1 - \exp(-2\tau)}{1 + \exp(-2\tau) + (n_1 - 1) \exp(-\tau)}\right) \\
&+ \log \left(1 + \exp(-2\tau) + (n_1 - 1) \exp(-\tau)\right) \\
&= \log(n_1 + 1) - o(1).
\end{aligned}
\end{equation}
C.3. Cycle graph. Now we consider the cycle graph. We will prove Eq. (10). The eigenvalues of the adjacency matrix of the cycle \( C_n \) take the form 
\[
\lambda_j = 2 \cos \left( \frac{2\pi j}{n} \right) \text{ for } j = 0, \ldots, n - 1. \]

Let \( N_{\tau,n,j} := \exp \left( -2\tau \cos \left( \frac{2\pi j}{n} \right) \right) \).

Then
\[
S(\varrho_{A(C_n)}) = 2\tau \sum_{j=0}^{n-1} \cos \left( \frac{2\pi j}{n} \right) N_{\tau,n,j} + \log \left( \sum_{j=0}^{n-1} N_{\tau,n,j} \right)
\]
(45)
\[
= 2\tau \frac{1}{n} \sum_{j=0}^{n-1} \cos \left( \frac{2\pi j}{n} \right) N_{\tau,n,j} + \log \left( \frac{1}{n} \sum_{j=0}^{n-1} N_{\tau,n,j} \right)
\]
\[
= 2\tau \frac{1}{n} \sum_{j=0}^{n-1} \cos \left( \frac{2\pi j}{n} \right) N_{\tau,n,j} + \log \left( \frac{1}{n} \sum_{j=0}^{n-1} N_{\tau,n,j} \right) + \log n.
\]

Now let us denote \( x_j := \frac{j}{n} \). We calculate
\[
\frac{1}{n} \sum_{j=0}^{n-1} N_{\tau,n,j} = \sum_{j=0}^{n-1} \frac{1}{n} \exp (-2\tau \cos (2\pi x_j))
\]
(46)
\[
\xrightarrow{n \to \infty} \int_0^1 \exp (-2\tau \cos (2\pi x)) \, dx = I_0(2\tau),
\]
where \( I_0(x) \) is the modified Bessel function of the first kind. Analogously we obtain
\[
\frac{1}{n} \sum_{j=0}^{n-1} \cos(2\pi x_j) N_{\tau,n,j} = \sum_{j=0}^{n-1} \frac{1}{n} \cos(2\pi x_j) \exp (-2\tau \cos (2\pi x_j))
\]
(47)
\[
\xrightarrow{n \to \infty} \int_0^1 \cos(2\pi x) \exp (-2\tau \cos (2\pi x)) \, dx = -I_1(2\tau).
\]

Summing up, as
\[
2\tau \frac{1}{n} \sum_{j=0}^{n-1} \cos \left( \frac{2\pi j}{n} \right) N_{\tau,n,j} + \log \left( \frac{1}{n} \sum_{j=0}^{n-1} N_{\tau,n,j} \right)
\]
(48)
\[
\xrightarrow{n \to \infty} 2\tau \frac{-I_1(2\tau)}{I_0(2\tau)} + \log \left( \frac{I_0(2\tau)}{I_0(2\tau)} \right),
\]
then for fixed \( \tau \) we have
\[
S(\varrho_{A(C_n)}) = \log n - 2\tau \frac{I_1(2\tau)}{I_0(2\tau)} + \log \left( \frac{I_0(2\tau)}{I_0(2\tau)} \right) + o(1).
\]
(49)

As a cycle is a 2-regular graph, then from Proposition \[2\] we have that the same result will be obtained for the Laplacian matrix of a cycle.

To see why Eq. (11) holds we note that as a cycle is a 2-regular graph, then \( L(C_n) = \frac{1}{2}L(C_n) \). Therefore it suffices to follow the proof of Eq.
knowing that the eigenvalues of the normalized Laplacian are $\lambda_j = 1 - \cos\left(\frac{2\pi j}{n}\right)$ for $j = 0, \ldots, n - 1$. 

[10]