

The von Neumann Entropy of Networks

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Outline

- Networks Anatomy: search for parameters encoding the structural properties
- A new structural parameter:

The von Neumann Entropy of Networks

- Definition and basic properties
- What does it tell us about networks ?
- What is it good for?

Networks Anatomy

- The structure of a network G is fully described by its *adjacency matrix* $A(G)$
- It is easier to consider a restricted set of structural characteristics:
 - degree distribution*
 - diameter*
 - clustering coefficient*
 - etc.*

Networks Anatomy

- Spectral Parameters: defined as functions of the spectrum of the *adjacency matrix* A or other matrices associated to the network
 - algebraic connectivity*
 - eigenvalue gap*
 - Estrada index*
 - etc.*

Von Neumann Entropy

- A state of a quantum mechanical systems is described by a density matrix ρ

ρ is a symmetric, positive definite

$$\text{Tr}(\rho) = 1$$

- The entropy of the state is given by

$$S(\rho) = -\text{Tr}(\rho \log_2 \rho)$$

Von Neumann Entropy

- It is a fundamental quantity in the study of *correlated systems* in quantum mechanics.
- It appears in the study of many applications ranging from the distribution of secret keys in cryptography to various nanoscale devices.
- Thus, to associate the von Neumann entropy to a network, we need to identify a map between networks and quantum states

Von Neumann Entropy

- We consider the map

$$\rho = \frac{L(G)}{\text{Tr}(\Delta(G))} \quad L(G) = \Delta(G) - A(G)$$

i.e. the density matrix associated to a network is given by the combinatorial laplacian, normalized by its trace.

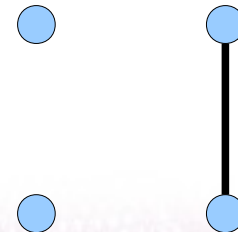
- Thus, for each network we can compute the von Neumann entropy!
- Which properties of the networks are encoded by the von Neumann entropy?

Basic properties

- *Theorem:*
 - Consider the set of networks with a given number of nodes n
 - The entropy is minimum for the graph with a single link and an arbitrary number of isolated nodes

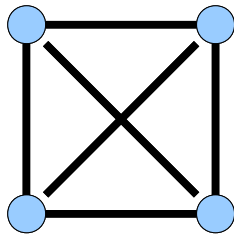
$$n = 4$$

$$S(G) = 0$$



Basic properties

- *Theorem:*
 - The entropy is maximum for the *complete graph*, $S(G) = \log_2(n - 1)$



- *Remark 1:* the entropy increases when the number of links increases.

Asymptotic Limit

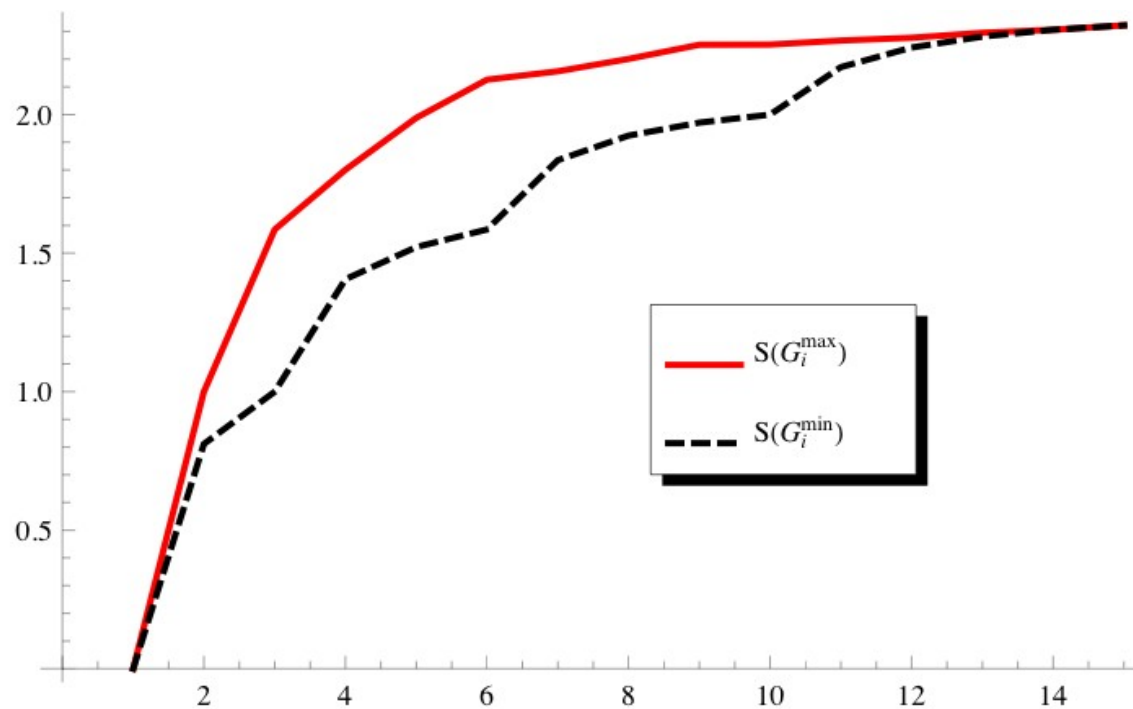
- Still consider the set of networks with a given number of nodes n , now n tends to infinity.
- *Theorem:* for a large number of nodes n , the entropy of a regular graph tends to the entropy of the complete graph, that results to be the maximum.
- *Theorem:* for a large number of nodes n , the entropy of the star graph tends to $1/2$ the entropy of the complete graph.

Asymptotic Limit

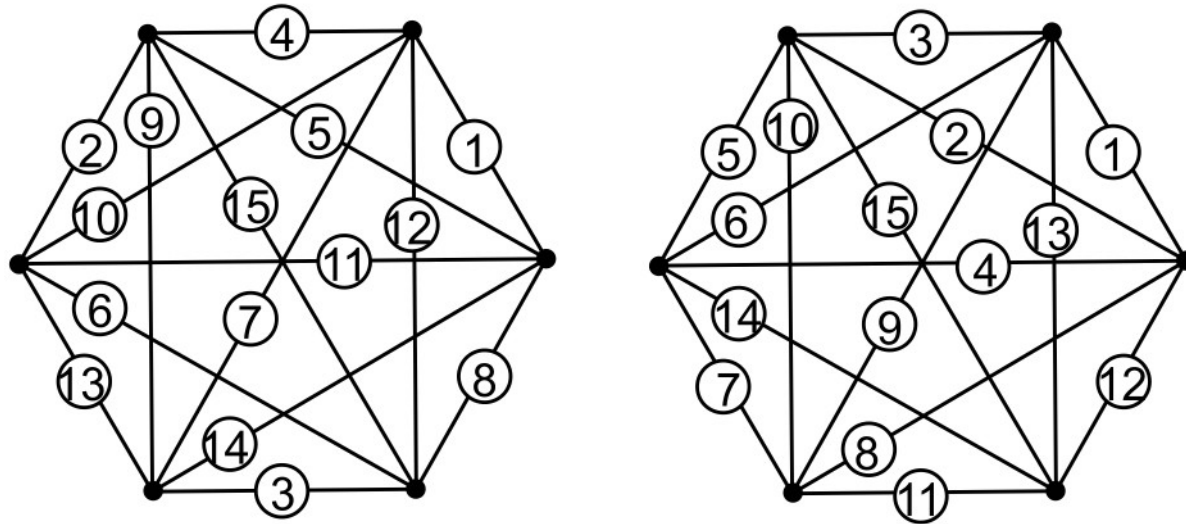
- *Remark 2:* the entropy tends to be larger for regular networks. It is a measure of regularity.

An Example

- Now we fix the number of nodes n and we add links in different ways. We consider the case $n=6$.



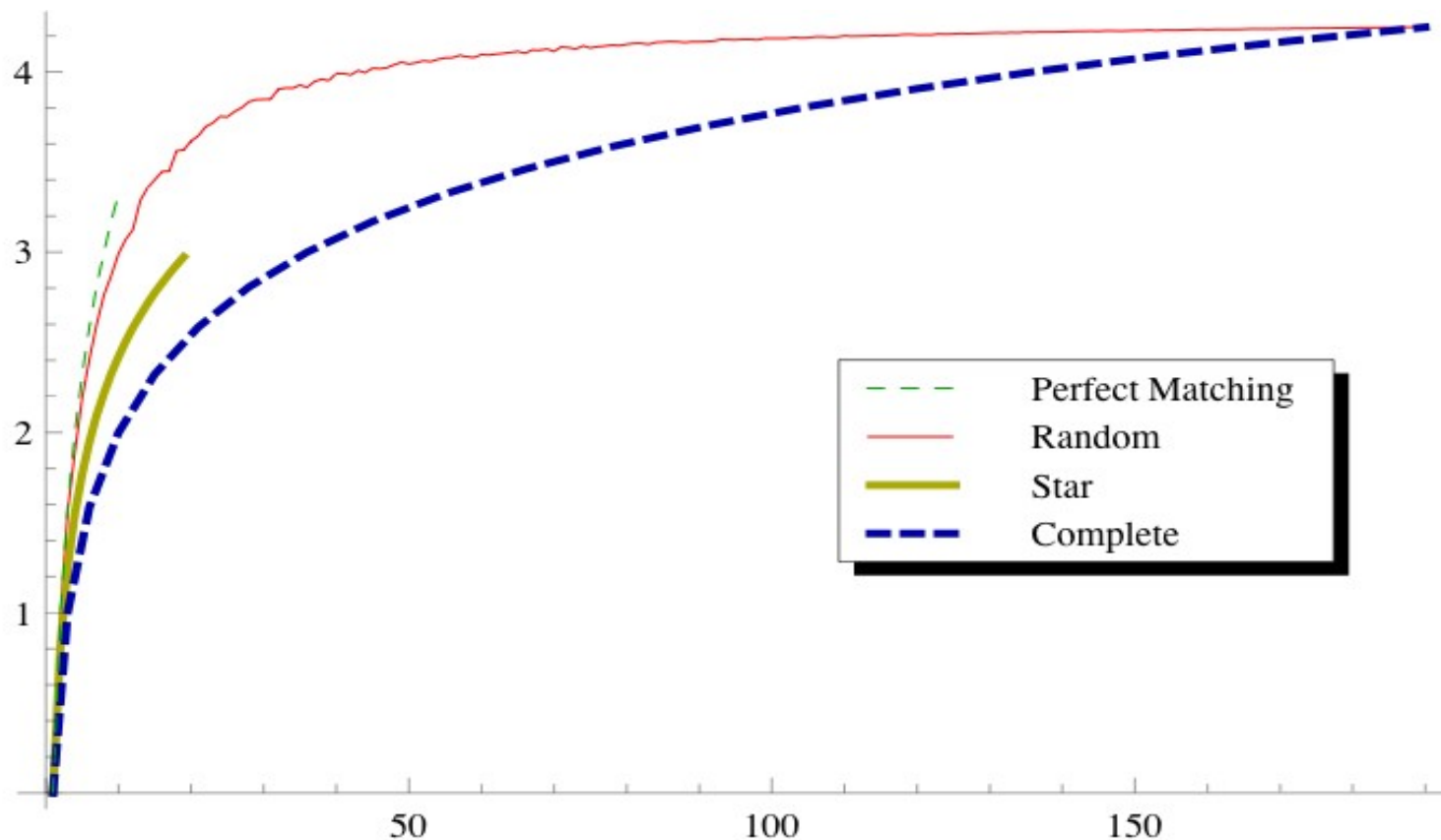
An Example



Remark 3: fixed the number of nodes and links, the entropy is minimum for networks containing large cliques and with a small number of components. Again we see that higher regularity implies higher entropy.

An Experiment

- We plot the entropy for various kinds of graphs as a function of the number of links



Summary

- The entropy increases when adding links to the network.
- The entropy increases with the regularity of the network.
- The entropy increases with the number of components.

Discussion

- Relation with *algebraic connectivity*:
Example: the complete graph and the cycle.
- Relation with the *eigenvalue gap*:
Example: the complete graph and the cycle.
- Is there a combinatorial definition for the von Neumann entropy of networks?
- Beyond cospectrality: determine families of coentropic but non-cospectral graphs.

Applications

- It is plausible that the von Neumann entropy is the first known information theoretic parameter to distinguish between scale-free graphs and random graphs.
- The von Neumann entropy is an efficiently computable parameter which may be used to control the algorithmic construction of networks where nodes/links are added sequentially under some constraints.
E.G. minimizing or maximizing the entropy itself.

Open problems

- Networks appear in many different areas of science. Do networks appearing in different areas show different behavior in relation to their von Neumann entropy?
- In general: what are the roles of the von Neumann entropy of networks?
- A recurrent principle in physics is the maximization of the entropy. Is a relatively small entropy proper of open complex systems?