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(G)* 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 symmetric and positive definite

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

- The entropy of the state is given by

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

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

$$\rho = \frac{L(G)}{\mathrm{Tr}(\Delta(G))} \qquad L(G) = \Delta(G) - A(G)$$

  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

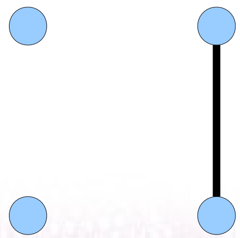
- *Theorem:*

  - 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

$n = 4$

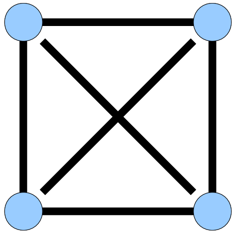
$$S(G) = 0$$



Basic properties

- *Theorem:*

  -The entropy is maximum for the *complete graph* K_n



$$S(G) = \log_2(n-1)$$

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

Basic properties

A bit more precise:

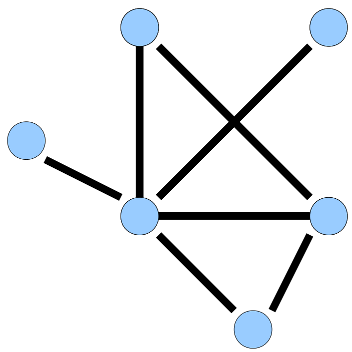
- *Theorem*:

For graphs G and $G' = G + \{x, y\}$,

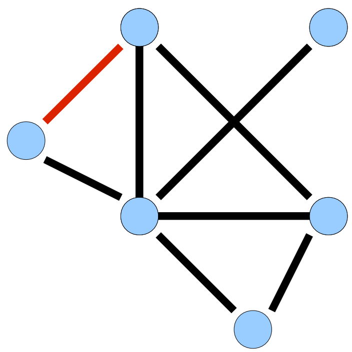
we have $$S(\rho_{G'}) \geq \frac{d_{G'} - 2}{d_{G'}} S(\rho_G)\ .$$

where: $d_G = \sum_{v \in V(G)} d(v)$

Basic properties



G



$G' = G + \{x, y\}$

Basic properties

- Comment:

  - For general density matrices, the entropy of a completely random state $\rho = \frac{1}{n} I_n$ is

$$S(\rho) = -\log_2 \frac{1}{n} = \log_2 n$$

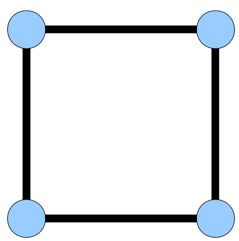
  - The analogue for graphs is given by K_n given that the spectrum of ρ_{K_n} is

$$\{ \frac{1}{n-1}^{[n-1]}, 0^{[1]} \}$$

Asymptotic Limit

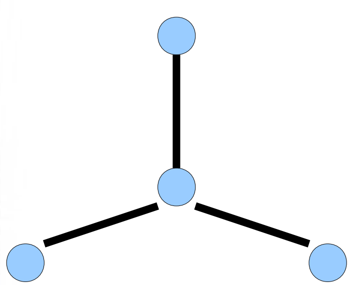
- Still consider the set of networks with a given number of nodes *n,* now *n* tends to infinity.
- *Theorem*: for a large number of nodes *n*, the entropy of a regular graph tends to the entropy of the complete graph, that results to be the maximum.
- *Theorem*: for a large number of nodes *n*, the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

Asymptotic Limit



$$if\ G \in \mathcal{G}_{n,d}$$

$$then\ \lim_{n\to\infty} \frac{S(G)}{S(K_n)} = 1$$



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

Asymptotic Limit

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

Asymptotic Limit

Generalizations:

- *Theorem:* Let *G* be a graph on *n* non-isolated vertices. If $\lim_{n\to\infty} \frac{R(G)}{\log_2 n} = 0$, then $\lim_{n\to\infty} \frac{S(G)}{S(K_n)} = 1$.

Where: $R(G) := \frac{1}{n} \sum_{i=1}^{n} \frac{\nu_i}{\bar{d}_G} \log_2 \frac{\nu_i}{\bar{d}_G}$

ν_i are the laplacian eigenvalues

$\bar{d}_G = \frac{1}{n} \sum_{v \in V(G)} d(v)$

Asymptotic Limit

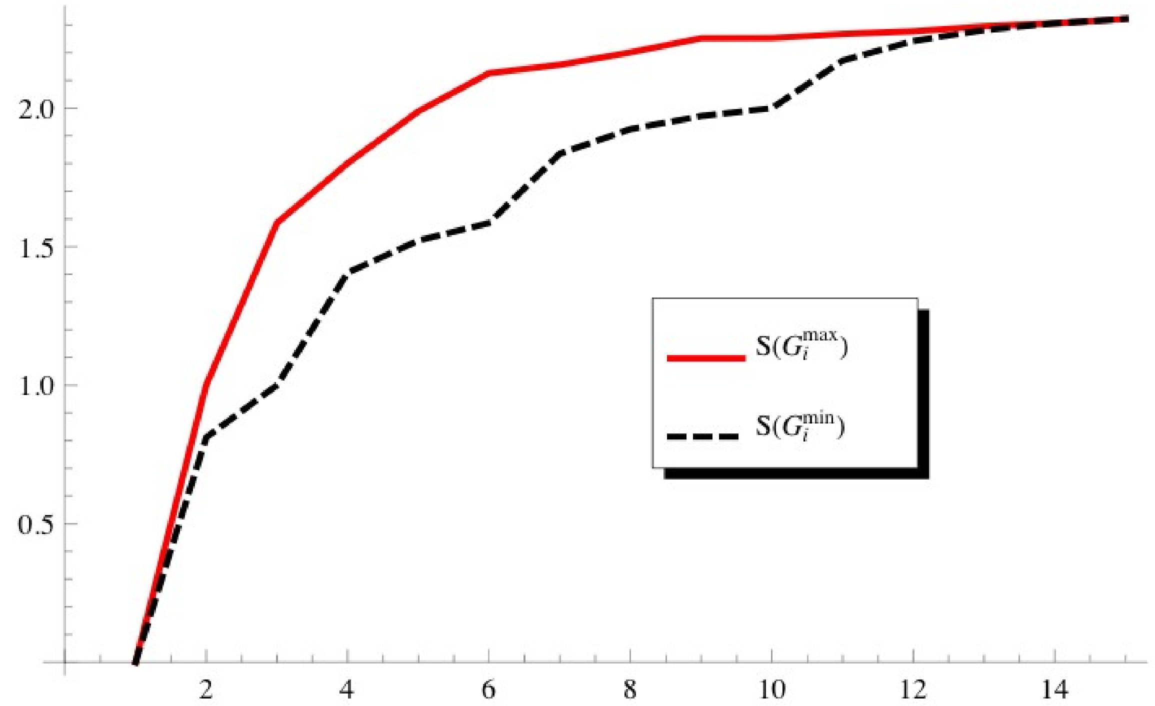
- *Theorem:* Let *G* be a graph on *n* non-isolated vertices such that one vertex is connected with all the other vertices and let

$$\lim_{n\to\infty} \bar{d}_G = d_\infty < \infty$$. Then

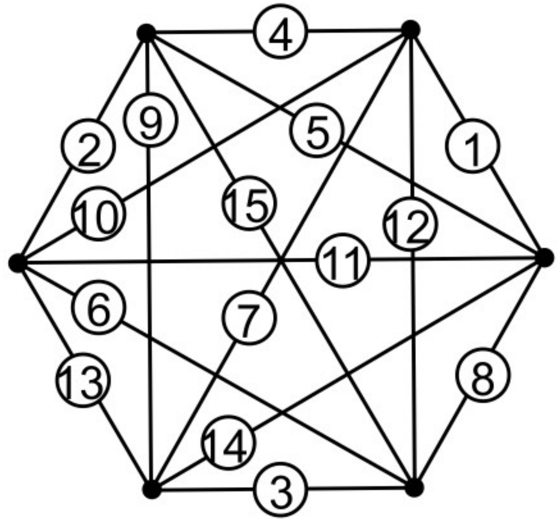
$$\lim_{n\to\infty} \frac{S(G)}{S(K_n)} \leq 1 - \frac{1}{d_\infty} .$$

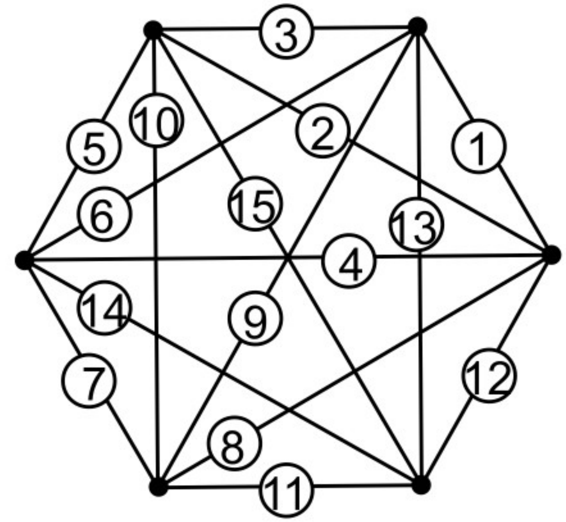
An Example

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



An Example





$$S(G_i^{\max}) \qquad\qquad S(G_i^{\min})$$

An Example

- The starting point is $K_2 \biguplus_{j=3}^{6} K_1^{(j)}$

- The ending point is $G_{15}^{\max} = G_{15}^{\min} = K_6$

- $G_{l(l-1)/2}^{\min} = K_l \biguplus_{j=1}^{6-l} K_1^{(j)}$

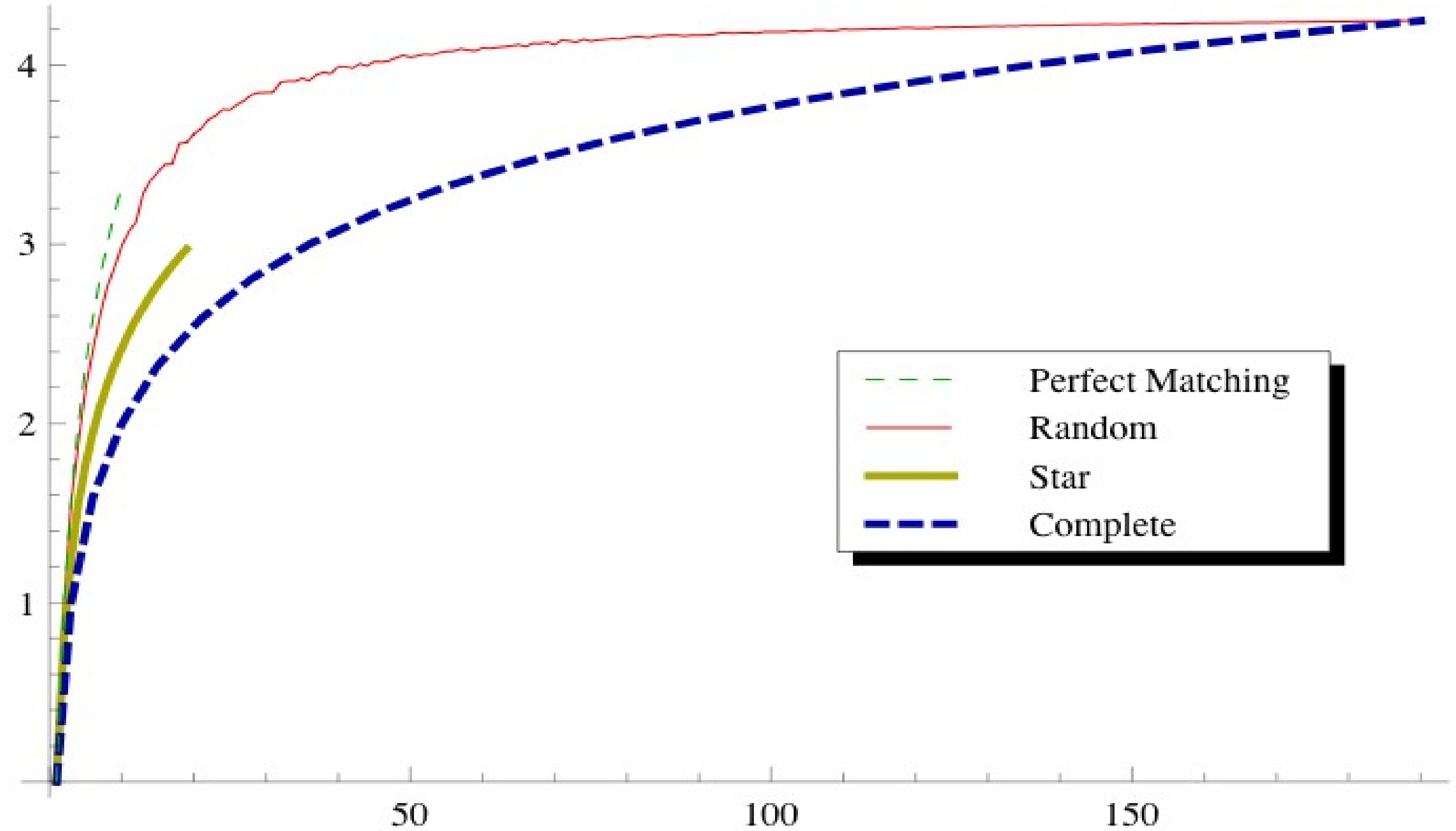
- $G_i^{\max}$ is a $i/3$-regular graph, for $i = 3, 6, 9, 12$

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.

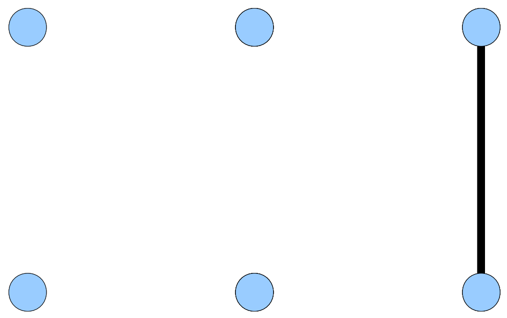
An Experiment

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



An Experiment

- *Perfect Matching* $M_{2e} \biguplus_{j=1}^{n-2e} K_1^{(j)}$



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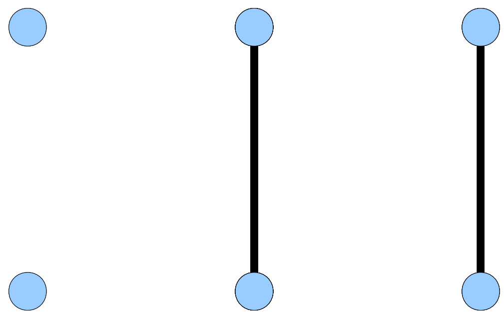

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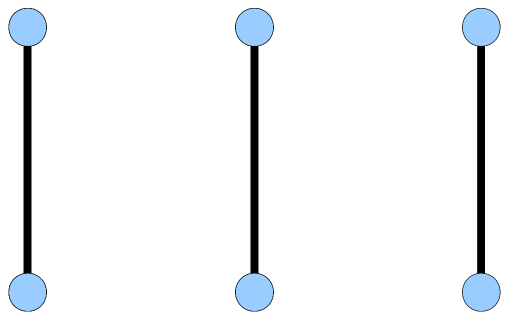

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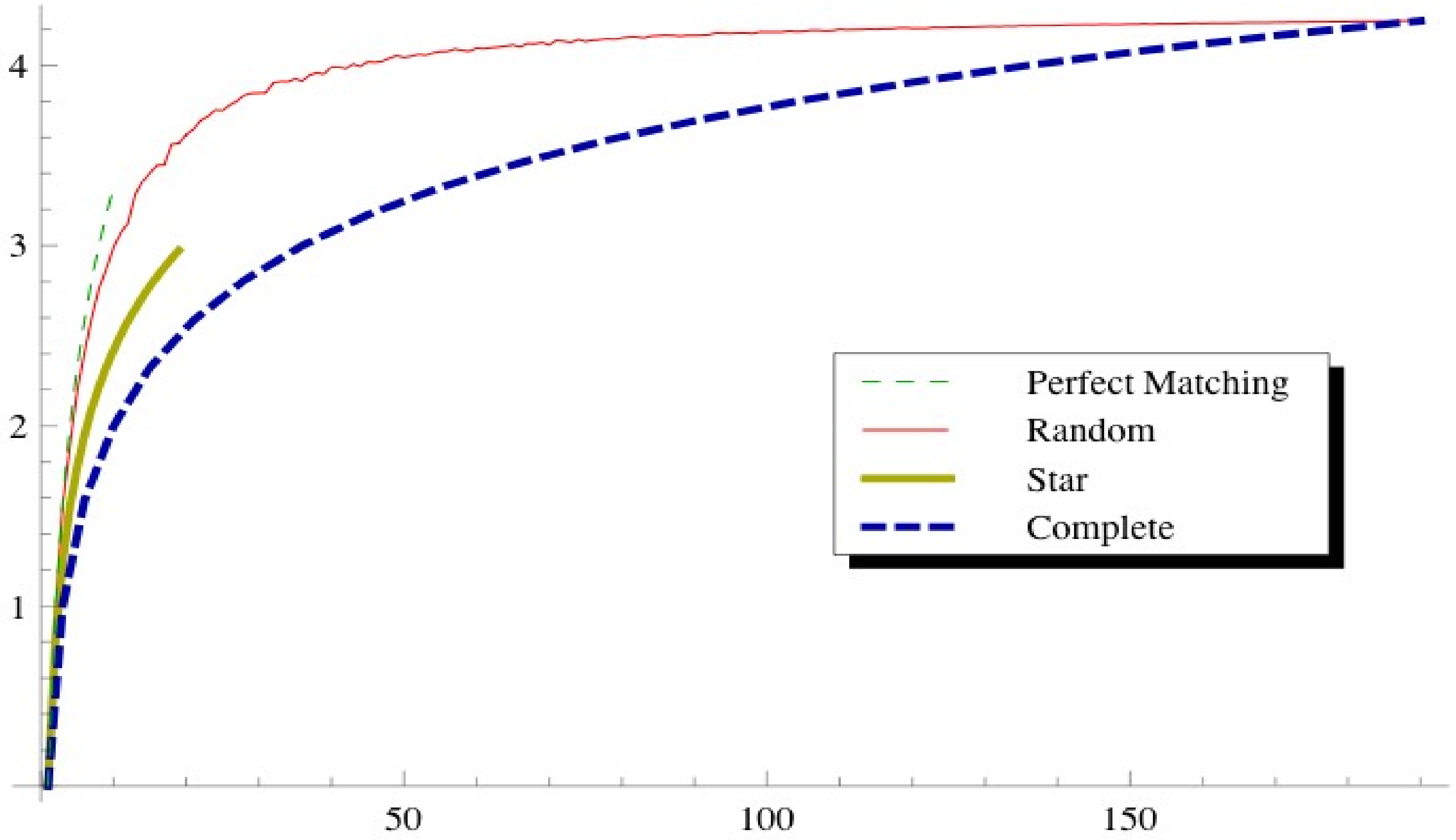

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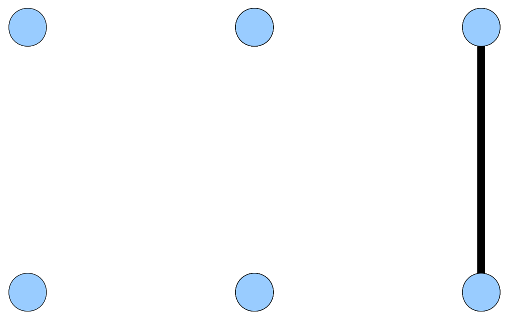
- *Random Graph* $R_{n,e}$



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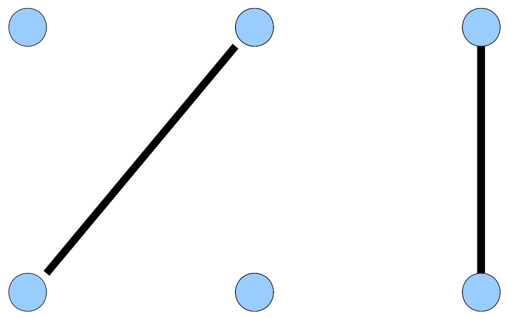

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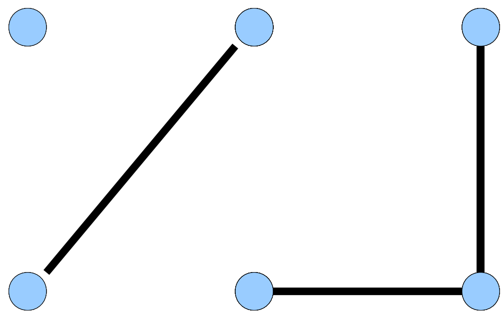

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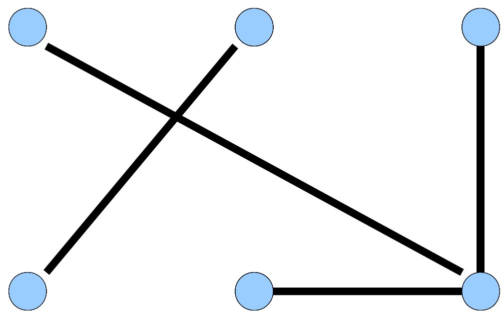

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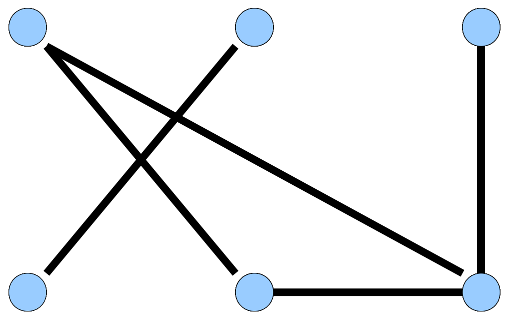

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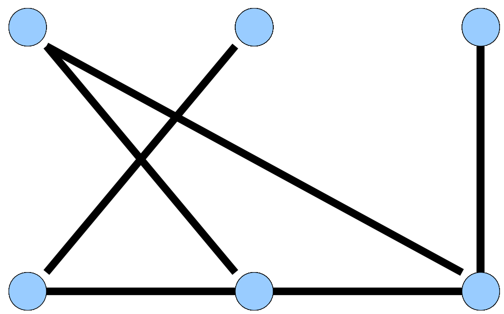

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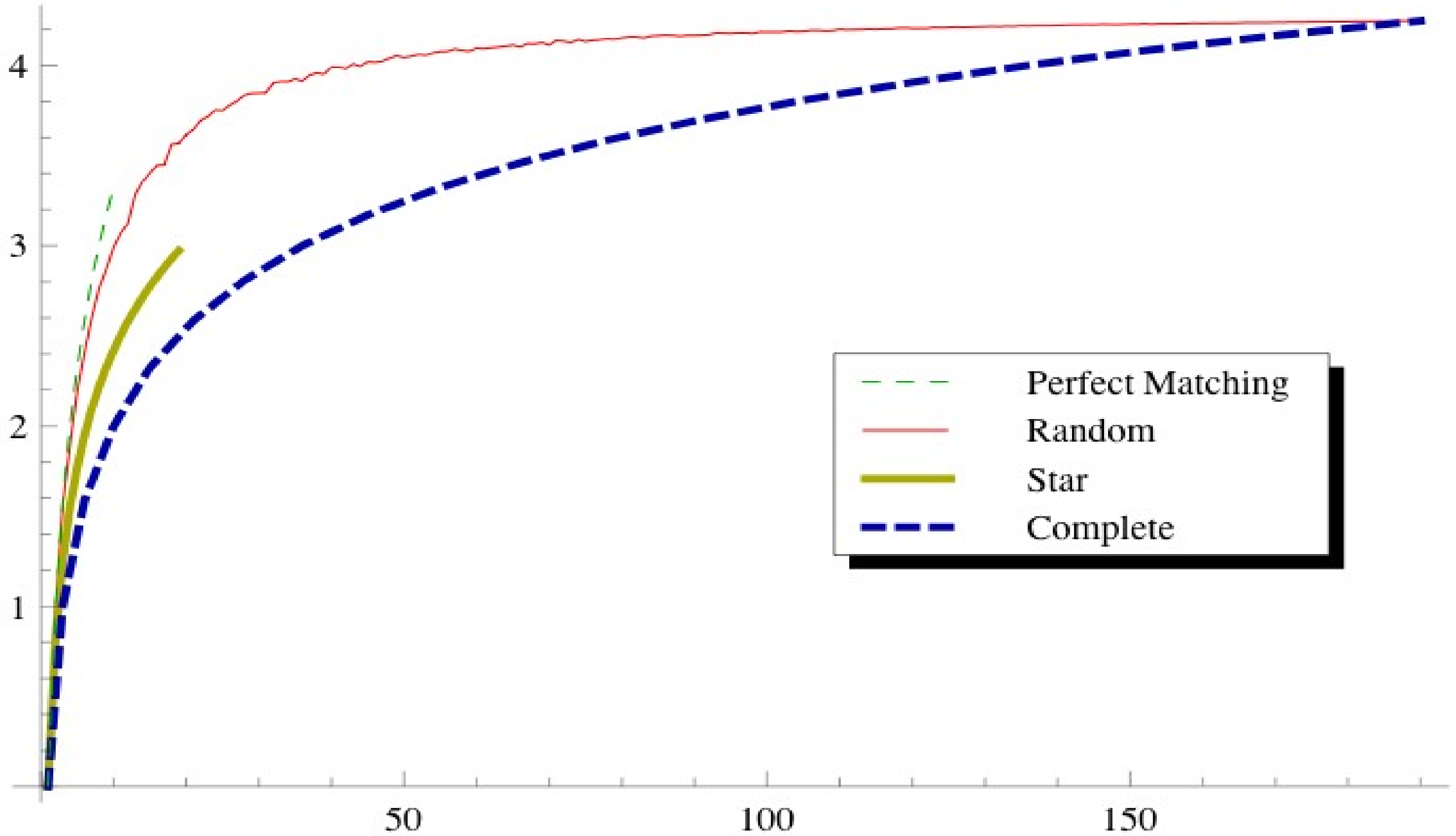
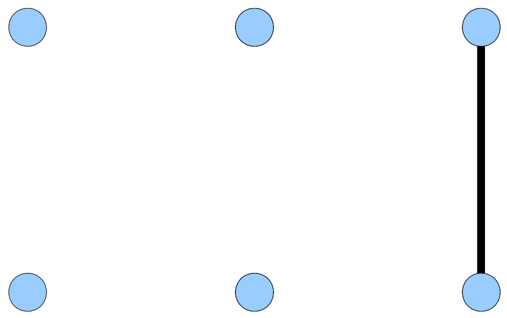


An Experiment

- *Star* $K_{1,(e+1)-1} \biguplus_{j=1}^{n-e-1} K_1^{(j)}$



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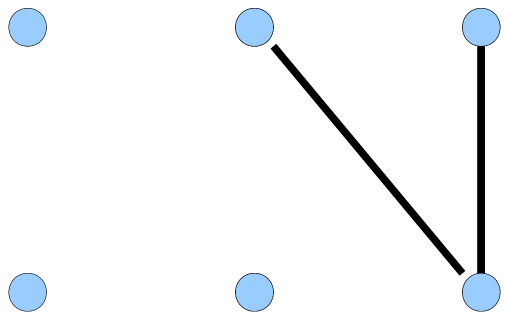

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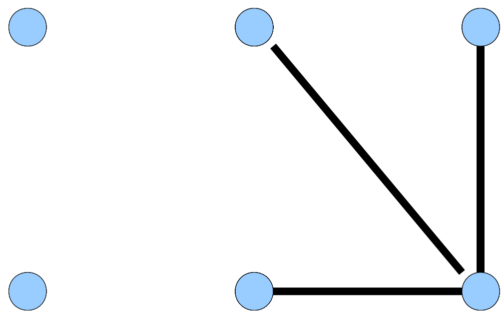

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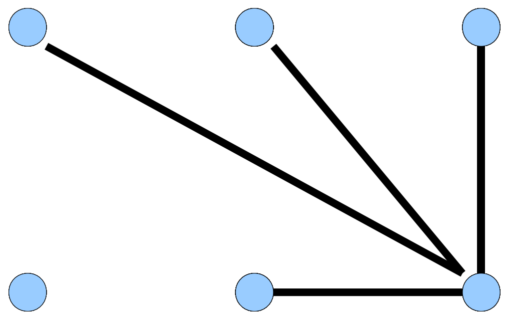

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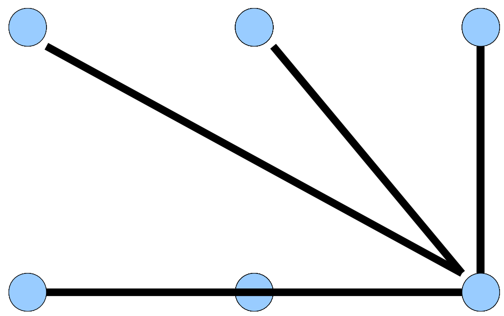

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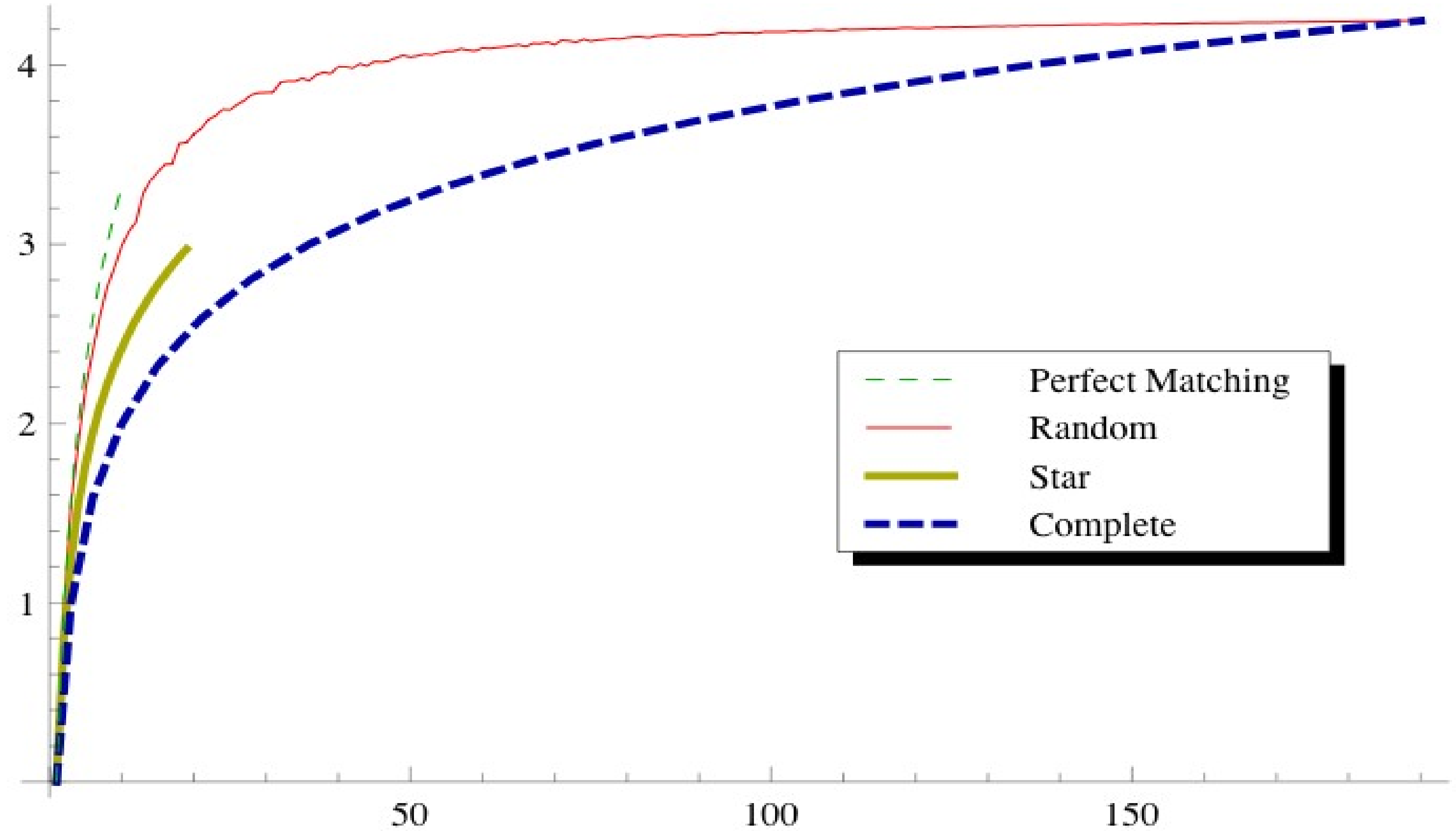
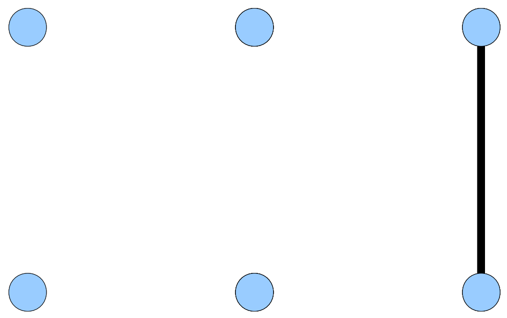


An Experiment

- *Complete* $K_m \biguplus_{j=1}^{n-m} K_1^{(j)}$



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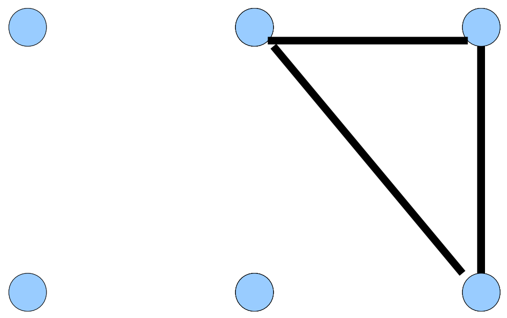

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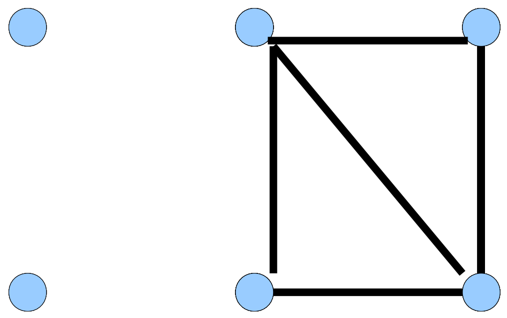

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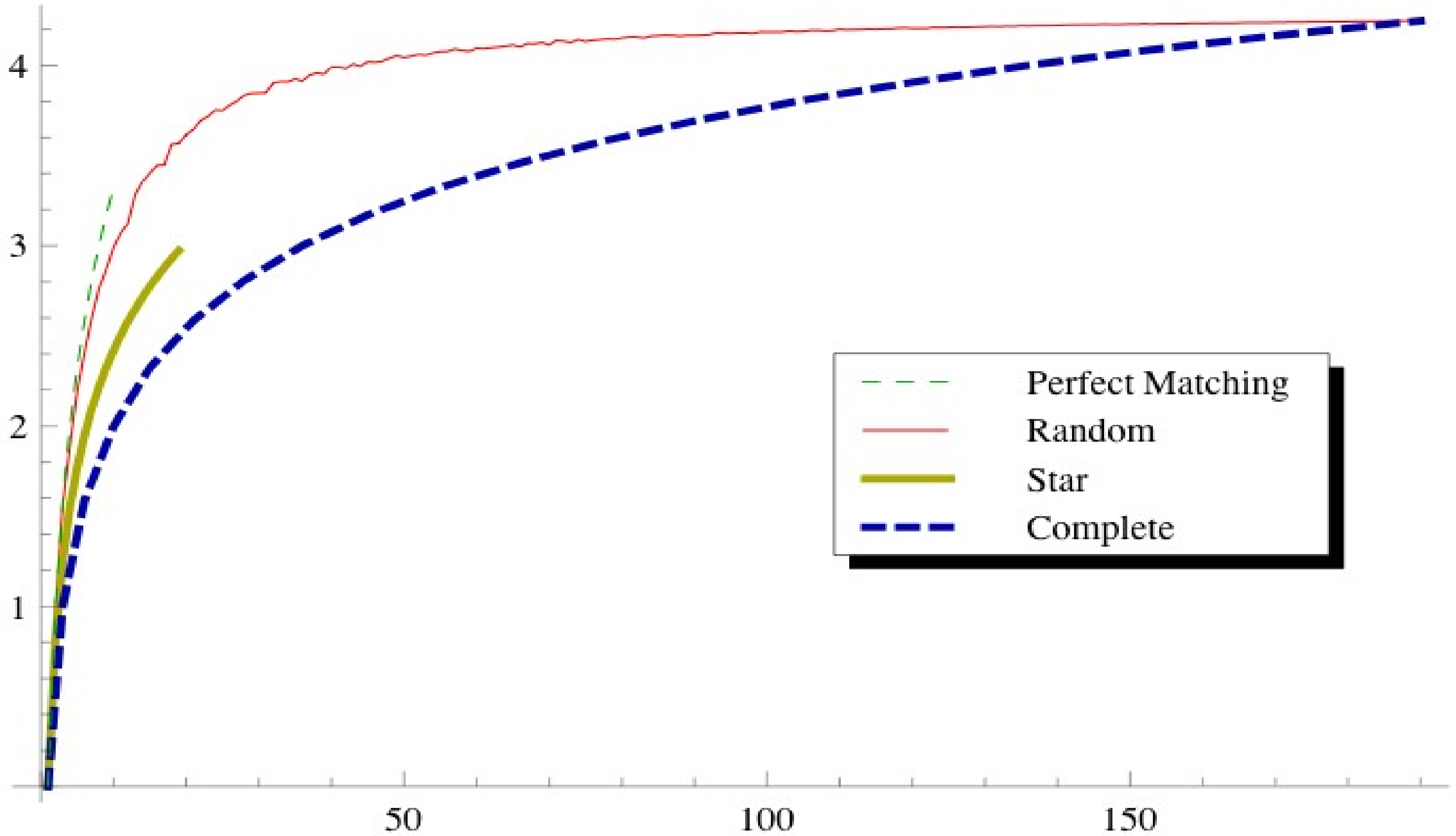

Summary

- 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?