7 Optimization in Complex Networks

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Abstract. Many complex systems can be described in terms of networks of interacting units. Recent studies have shown that a wide class of both natural and artificial nets display a surprisingly widespread feature: the presence of highly heterogeneous distributions of links, providing an extraordinary source of robustness against perturbations. Although most theories concerning the origin of these topologies use growing graphs, here we show that a simple optimization process can also account for the observed regularities displayed by most complex nets. Using an evolutionary algorithm involving minimization of link density and average distance, four major types of networks are encountered: (a) sparse exponential-like networks, (b) sparse scale-free networks, (c) star networks and (d) highly dense networks, apparently defining three major phases. These constraints provide a new explanation for scaling of exponent about -3. The evolutionary consequences of these results are outlined.

7.1 Introduction

Many essential features displayed by complex systems, such as memory, stability and homeostasis emerge from their underlying network structure [26, 14]. Different networks exhibit different features at different levels but most complex networks are extremely sparse and exhibit the so-called small-world phenomenon [28]. An inverse measure of sparseness, the so-called network density, is defined as

$$\rho = \frac{\langle k \rangle}{n-1} \tag{7.1}$$

where n is the number of vertices of the network and $\langle k \rangle$ is its average degree. For real networks we have $\rho \in [10^{-5}, 10^{-1}]$[3].

It has been shown that a wide range of real networks can be described by a degree distribution $P(k) \sim k^{-\gamma}\phi(k/\xi)$ where $\phi(k/\xi)$ introduces a cut-off at some characteristic scale ξ. Three main classes can be defined [2]. (a) When ξ is very small, $P(k) \sim \phi(k/\xi)$ and thus the link distribution is single-scaled. Typically, this would correspond to exponential or Gaussian distributions; (b) as ξ grows, a power law with a sharp cut-off is obtained; (c) for large ξ, scale-free nets are observed. The last two cases have been shown to be widespread and

[3] Statistics performed on Table I in [5]

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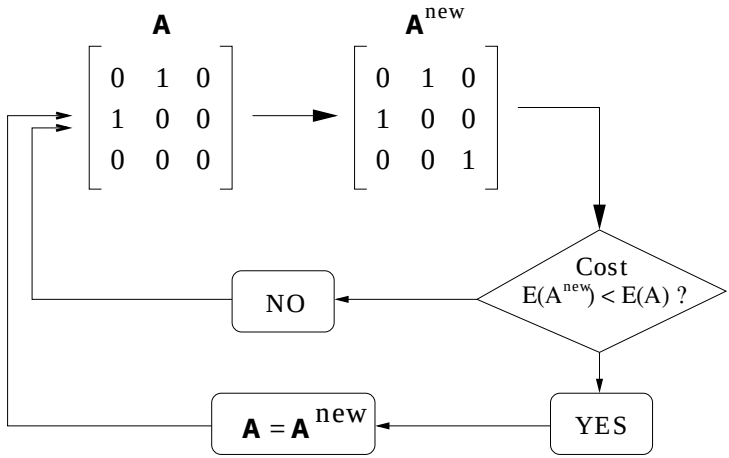

Fig. 7.1. Basic scheme of the minimization algorithm. Starting from a given adjacency matrix **A** the algorithm performs a change in a small number of bits (specifically, with probability ν, each a_{ij} can flip). The energy function e is then evaluated and the new matrix is accepted provided that a lower cost is achieved. Otherwise, we start again with the original matrix. At the beginning, **A** is set up with a fixed density $\rho(0)$ of ones

their topological properties have immediate consequences for network robustness and fragility [5]. The three previous scenarios are observed in: (a) power grid systems and neural networks [2], (b) protein interaction maps [12], metabolic pathways [13] and electronic circuits [16] and (c) Internet topology [13, 8], scientific collaborations [20] and [17] lexical networks.

7.2 Network Optimization

Scale-free nets are particularly relevant due to their extremely high homeostasis against random perturbations and fragility against removal of highly connected nodes[1]. These observations have important consequences, from evolution to therapy [12]. One possible explanation for the origin of the observed distributions would be the presence of some (decentralized) optimization process.

Network optimization is actually known to play a leading role in explaining allometric scaling in biology [29, 7, 3] and has been shown to be a driving force in shaping neural wiring at different scales [9, 18] (see also [6]). In a related context, local and/or global optimization has been also shown to provide remarkable results within the context of channel networks [22]. By using optimality criteria linking energy dissipation and runoff production, the fractal properties in the model channel nets were essentially indistinguishable from those observed in nature. Figure 7.2 displays different optimal transportation networks.

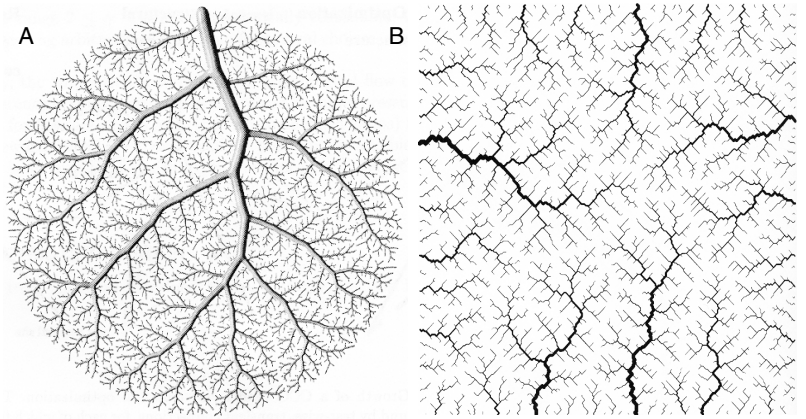

Fig. 7.2. Optimal transport networks in biology (**A**) and geomorphology (**B**). **A.** An optimal tree structure that has been obtained for a vascular system on a two dimensional perfusion area [7]. **B.** An optimal river basin network (also displaying tree structure) that has been generated by minimizing energy expenditure [22]

Several mechanisms of network evolution lead to scale-free structures within the context of complex networks in which the only relevant elements are vertices and connections [4]. Optimization has not been found to be one of them [5]. In this context, it was shown that (Metropolis-based) minimization of both vertex-vertex distance and link length (*i.e.* Euclidean distance between vertices)[15] can lead to the small-world phenomenon and hub formation. This view takes into account Euclidean distance between vertices. Here we show how minimizing both vertex-vertex distance and the number of links leads (under certain conditions) to the different types of network topologies depending on the weight given to each constraint. These two constraints include two relevant aspects of network performance: the cost of physical links between units and communication speed among them.

7.3 The Optimization Algorithm

For the sake of simplicity, we take an undirected graph having a fixed number of nodes n and links defined by a binary adjacency matrix $A = \{a_{ij}\}$, $1 \leq i, j \leq n$. Given a pair of vertices i and j, $a_{ij} = 1$ if they are linked ($a_{ij} = 0$ otherwise) and D_{ij} is the minimum distance between them. At time $t = 0$, we have a randomly wired graph (i.e. a Poisson degree distribution) in which two given nodes are connected with some probability p. The energy function of our optimization algorithm is defined as

$$E(\lambda) = \lambda d + (1 - \lambda)\rho$$

where $0 \leq \lambda, d, \rho \leq 1$. λ is a parameter controlling the linear combination of d and ρ. The normalized number of links, ρ is defined in terms of a_{ij} as

$$\rho = \frac{1}{\binom{n}{2}} \sum_{i<j} a_{ij}$$

and it is equivalent to (7.1). The normalized vertex-vertex distance, d, is defined as $d = D/D^{linear}$ being

$$D = \frac{1}{\binom{n}{2}} \sum_{i<j} D_{ij}$$

the average minimum vertex-vertex distance and $D^{linear} = (n+1)/3$ the maximum value of D that can be achieved by a connected network, that is, that of a linear graph (see Appendix). We define a linear graph as a graph having 2 vertices with degree 1 and $n-2$ vertices with degree 2[4]. A graph whose adjacency matrix satisfies

$$a_{ij} = \begin{cases} 1 \text{ if } |i-j| = 1 \\ 0 \text{ otherwise} \end{cases} \tag{7.2}$$

is a linear graph. Such a graph has the maximum average vertex-vertex distance that can be achieved by a connected graph of order n (see Appendix).

The minimization of $E(\lambda)$ involves the simultaneous minimization of distance and number of links (which is associated to cost). Notice that minimizing $E(\lambda)$ implies connectedness (*i.e.* finite vertex-vertex distance) except for $\lambda = 0$, where it will be explicitly enforced.

The minimization algorithm proceeds as follows. At time $t = 0$, the network is set up with a density $\rho(0)$ following a Poissonian distribution of degrees (connectedness is enforced). At time $t > 0$, the graph is modified by randomly changing the state of some pairs of vertices. Specifically, with probability ν, each a_{ij} can switch from 0 to 1 or from 1 to 0. The new adjacency matrix is accepted if $E(\lambda, t+1) < E(\lambda, t)$. Otherwise, we try again with a different set of changes. The algorithm stops when the modifications on $A(t)$ are not accepted T times in a row. The minimization algorithm is a simulated annealing at zero temperature. Figure 7.1 describes the minimization algorithm. Hereafter, $n = 100$[5], $T = \binom{n}{2}$[6], $2/\binom{n}{2}$[7] and $\rho(0) = 0.2$.

[4] It can be easily shown through induction on n that such a graph is connected and has no cycles.

[5] Higher values of n were very time consuming. The critical part of the algorithm is the calculation of d which has cost $\Theta(n\rho\binom{n}{2})$, that is, $\Omega(n^2)$ and $O(n^3)$. Faster calculation implies performing an estimation of d on a random subset of vertices or 1st and 2nd neighbors [21] that happened to be misleading.

[6] Intended for expecting that every pair of vertices has been allowed to change its state at least once.

[7] We define the number of changes in the adjacency matrix between generations as $c = |\{a_{ij}(t+1) | i < j \text{ and } a_{ij}(t+1) \neq a_{ij}(t)\}|$. Let $d(t)$ and $\rho(t)$ be respectively the distance and the density at time t. If $c = 1$ then $d(t+1) < d(t)$ and $\rho(t+1) = \rho(t)$ is impossible. If $c > 1$ then $d(t+1) < d(t)$ with $\rho(t+1) = \rho(t)$ is allowed. Thereafter ν is set to enforce $E[c] = 2 > 1$.

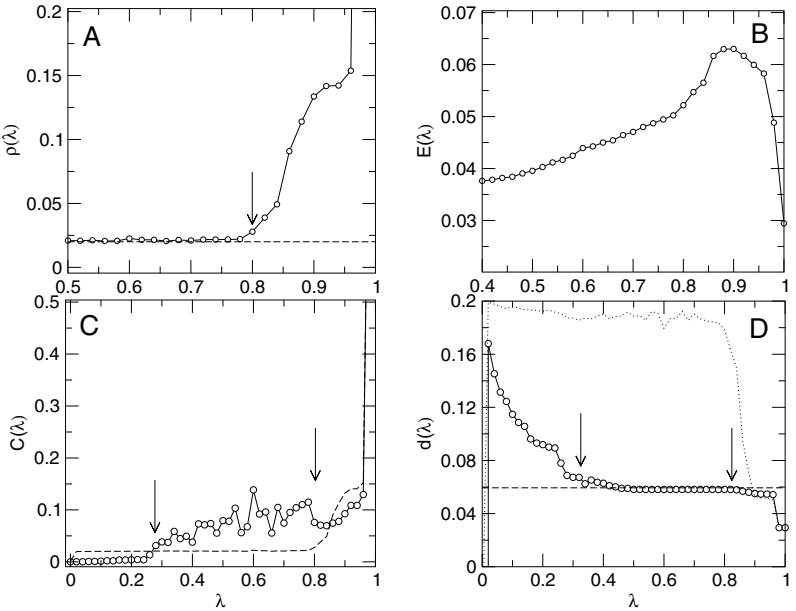

Fig. 7.3. Density (**A**), energy (**B**), clustering coefficient (**C**) and distance (**D**) as a function of λ. Averages over 50 optimized networks with $n = 100$, $T = \binom{n}{2}$, $\nu = 2/\binom{n}{2}$ and $\rho(0) = 0.2$ are shown. **A:** the optimal network becomes a complete graph for λ close to 1. The density of a star network, $\rho_{star} = 2/n = 0.02$ is shown as reference (*dashed line*). The clustering coefficient of a Poissonian network $C_{random} = \langle k \rangle/(n-1)$ is shown as reference in **C**. Notice that $C_{random} \approx \rho$. The normalized distance of a star network is (see Appendix), $d_{star} = 6(n-1)/(n(n+1)) = 0.058$ (*dashed line*) and that of a Poissonian network, $d_{random} = \log n/\log \langle k \rangle$ (*dotted line*) are shown for reference in **D**

We define the degree entropy on a certain value of λ as

$$H(\{p_k\}) = -\sum_{k=1}^{n-1} p_k \log p_k$$

where p_k is the frequency of vertices having degree k and $\sum_{k=1}^{n-1} p_k = 1$. This type of informational entropy will be used in our characterization of the different phases[8].

Some of the basic average properties displayed by the optimized nets are shown against λ in Fig. 7.3. These plots, together with the degree entropy in Fig. 7.4 suggest that four phases are present, separated by three sharp transitions at $\lambda_1^* \approx 0.25$, $\lambda_2^* \approx 0.80$ and $\lambda_3^* \approx 0.95$ (see arrows in Fig. 7.3). The second one

[8] Entropy measures of this type have been used in characterizing optimal channel networks and other models of complex systems (see [24]) although they are typically averaged over time.

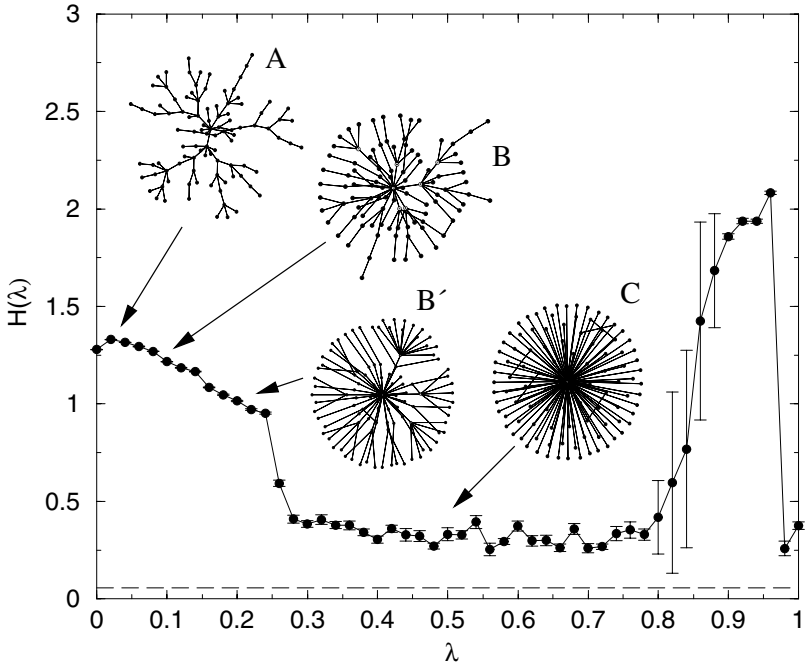

Fig. 7.4. Average (over 50 replicas) degree entropy as a function of λ with $n = 100$, $T = \binom{n}{2}$, $\nu = 2/\binom{n}{2}$ and $\rho(0) = 0.2$. Optimal networks for selected values of λ are plotted. The entropy of a star network, $H_{star} = \log n - [(n-1)/n]\log(n-1) = 0.056$ is provided as reference (dashed line). **A:** an exponential-like network with $\lambda = 0.01$. **B:** A scale-free network with $\lambda = 0.08$. Hubs involving multiple connections and a dominance of nodes with one connection can be seen. **C:** a star network with $\lambda = 0.5$. **B':** a intermediate graph between **B** and **C** in which many hubs can be identified

separates sparse nets from dense nets and fluctuations in $H(\lambda_3^*)$ are specially high. $\rho(\lambda), C(\lambda) \approx 1$ for $\lambda > \lambda_3^* \approx 0.95$. For $\lambda = 0$ and $\lambda = 1$ a Poissonian and a complete ($\rho(\lambda) = 1$) network are predicted, respectively.

7.4 Optimal Degree Distributions

When taking a more careful look at the sparse domain $(0, \lambda_2^*)$, three non-trivial types of networks are obtained as λ grows:

a. Exponential networks, i. e. $P_k \sim e^{-k/\xi}$.
b. Truncated scale-free networks, i. e. $P_k \sim k^{-\gamma} e^{-k/\xi}$ with $\gamma = 3.0$ and $\xi \approx 20$ (for $n = 100$).
c. Star network phase ($\lambda_1^* < \lambda < \lambda_2^*$) *i.e.* a central vertex to which the rest of the vertices are connected to (no other connections are possible). Here,

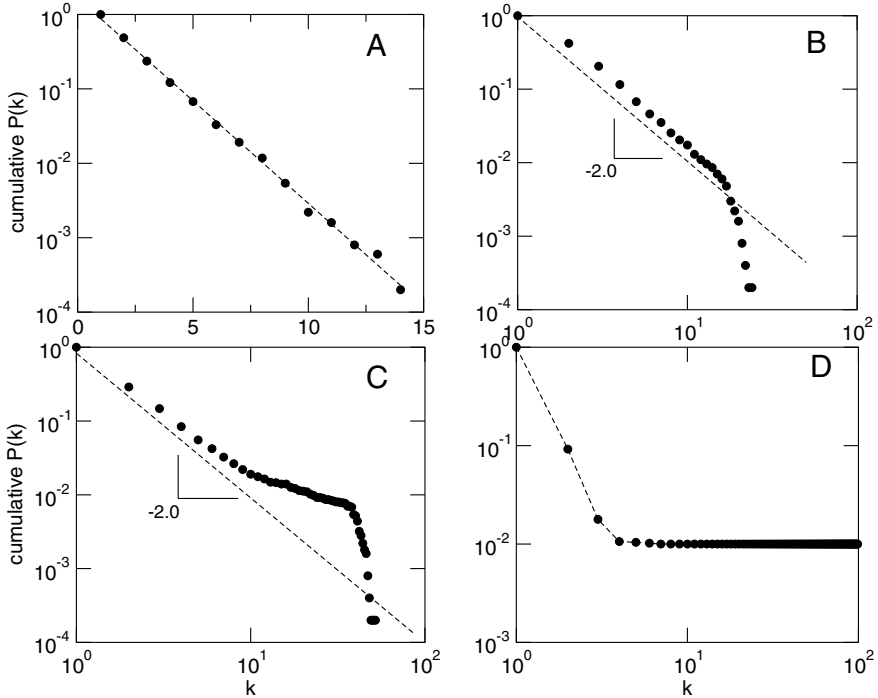

Fig. 7.5. Selected cumulative degree distributions of networks obtained minimizing $E(\lambda)$. Every distribution is an average over 50 optimized networks with $n = 100$, $T = \binom{n}{2}$, $\nu = 2/\binom{n}{2}$ and $\rho(0) = 0.2$. **A:** an exponential-like distribution for $\lambda = 0.01$. **B:** a power distribution with exponent $\gamma = 2.0$ for $\lambda = 0.08$ (with a sharp cutoff at $\xi \approx 20$). **C:** $\lambda = 0.20$. **D:** $\lambda = 0.50$ (almost an star graph)

$$p_k = \frac{n-1}{n}\delta_{k,1} + \frac{1}{n}\delta_{k,n-1} \tag{7.3}$$

A star graph has the shortest vertex-vertex distance between vertices among all the graphs having a minimal amount of links (see Appendix). Non-minimal densities can be compensated with a decrease in distance, so pure star networks are not generally obtained.

The distributions of (a-c) types and that of a dense network are shown in Fig. 7.5. A detailed examination of the transition between degree distributions reveals that hub formation explains the emergence of (b) from (a), hub competition (b') precedes the emergence of a central vertex in (c). The emergence of dense graphs from (c) consists of a progressive increase in the average degree of non-central vertices and a sudden loss of the central vertex. The transition to the star net phase is sharp. Figure 7.4 shows $\langle H(\lambda)\rangle$ along with plots of the major types of networks. It can be seen that scale-free networks (b) are found close to λ_1^*. The cumulative exponent of such scale-free networks is two and thus

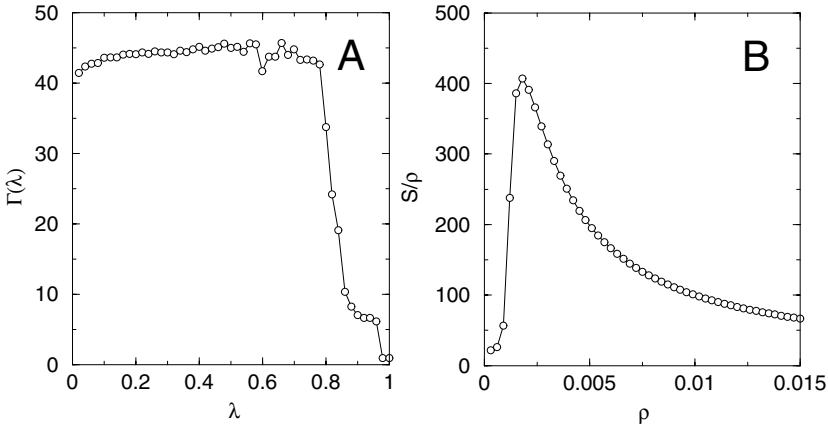

Fig. 7.6. A. The function $\Gamma(\lambda) = (1 - d(\lambda))/\rho(\lambda)$ for the minimum energy configurations. **B.** The cost function S/ρ versus ρ for the Poissonian model

$\gamma = 3.0$, the same that it would be expected for a random network generated with the Barabási-Albert model [4].

Our scenario suggests that preferential attachment networks might emerge at the boundary between random attachment networks (a) and forced attachment (*i.e.* every vertex connected to a central vertex) networks (c) and points that optimization can explain the selection of preferential attachment strategies in real complex networks. In our study, exponential-like distributions appear when distance is minimized under high density pressure, in agreement with the study by Amaral and co-workers on classes of small-world networks [2]. This might be the case of the power grid and of neural networks [2]. If linking cost decreases sufficiently, cliquishness becomes an affordable strategy for reducing vertex-vertex distance. Consistently, graphs tend to a complete graph for high values of λ. The Watts model [28] is a non-trivial example of what cliquishness (i.e. high clustering) can do for smallwordness. High clustering favours small-worldness (as seen for $\lambda \geq \lambda_2^*$) but it is not the only mechanism [10].

We have seen the different optimal topologies depending on the value of λ. We are aimed at defining an absolute measure of optimality depending on λ we can use for ranking the different topologies. We define

$$\Gamma(\lambda) = \frac{1 - d(\lambda)}{\rho(\lambda)} \tag{7.4}$$

as such measure (Fig. 7.6A). A sharp transition from sparse to dense networks is clearly observed for $\lambda \approx 0.8$. According to Fig. 7.6A, the topology ranking becomes,

1. Star networks.
2. Scale-free networks.

3. Exponential networks.
4. Dense networks.

See the Appendix section for a summary of the basic features of the trivial topologies appearing in our study.

A simpler version of the previous scenario appears in the context of Poissonian graphs, where we define the optimality measure as S/ρ, where S is the number of vertices of the largest connected component and ρ is both the expected network density and the probability that a random pair of vertices are linked. Again, the maximum divides networks into disconnected networks and connected networks at high link expense (Fig. 7.6B). $\rho \approx 0.8$ divides low cost strategies from high cost strategies as $\lambda = 0.8$ does in Fig. 7.6A. Notice that the transition is smooth for the former and sharp for the latter. The Poissonian scenario shows the optimization principles that may guide networks in early stages to remain close to the connectedness transition. Once enough connectedness is achieved, networks may be guided by (7.4) or particular values of λ depending on the system.

7.5 Discussion

The network previous results and our conjecture concerning optimization in complex nets requires explaining why star graphs are not found in nature. Different constraints can be restricting the access of star graphs to real systems. Let us list some of them:

- Randomness. The evolution of the topology as λ grows suggests a transition from disorder (exponential degree distribution) to order (star degree distribution).
- Diversity. The number of different star graphs that can be formed with n vertices is n whereas it explodes for exponential and power distributions.
- Robustness. Removing the central hub leaves $n-1$ connected components, which is the worst case situation.

Whether or not optimization plays a key role in shaping the evolution of complex networks, both natural and artificial, is an important question. Different mechanisms have been suggested to explain the emergence of the striking features displayed by complex networks. Most mechanisms rely on preferential attachment-related rules, but other scenarios have also been suggested [25, 27] in which external parameters have to be tuned. When dealing with biological networks, the interplay between emergent properties derived from network growth and selection pressures has to be taken into account. As an example, metabolic networks seem to result from an evolutionary history in which both preferential attachment and optimization are present. The topology displayed by metabolic networks is scale-free, and the underlying evolutionary history of these nets suggests that preferential attachment might have been involved [11]. Early in the

evolution of life, metabolic nets grew by adding new metabolites, and the most connected are actually known to be the oldest ones. On the other hand, several studies have revealed that metabolic pathways have been optimized through evolution in a number of ways. This suggests that the resulting networks are the outcome of both contributions, plus some additional constraints imposed by the available components to the evolving network [19, 23]. In this sense, selective pressures might work by tuning underlying rules of net construction. This view corresponds to Kauffman's suggestion that evolution would operate by taking advantage of some robust, generic mechanisms of structure formation [14].

Appendix

Throughout this paper, different trivial topologies have appeared. Table 7.1 summarizes their features indicating the value of λ at which they appear. Although this paper is concerned with what happens for $\lambda \geq 0$, notice that the linear graph is the expected outcome for $\lambda < 0$, since it implies distance maximization and density minimization. The remaining of this section is devoted to proof that a linear graph and a star graph have the maximum finite distance and the minimum distance (with the constraints of connectedness and having the smallest amount of edges).

A linear graph is a graph having the maximum finite distance or in other words, it is the connected graph having the maximum distance. We will proof it through induction on n. For $n = 2$, there is only one possible connected graph, which trivially has the maximum distance. All linear graphs having the same amount of vertices have the same average vertex-vertex distance. If the graph in (7.2) has the maximum distance for n vertices, will it still be the longest for $n+1$ vertices? Assuming that the graph in (7.2) is the longest for n vertices, the longest graph of $n+1$ vertices has to be formed by the longest graph of order n and a new a vertex linked to one of the n existing vertices. Here we define the total vertex-vertex distance as

$$D_n = \sum_{i<j} D_n(i,j) \tag{7.5}$$

Table 7.1. Different trivial topologies with density (i.e. normalized amount of links) ρ, average vertex-vertex distance D, clustering coefficient C, degree distribution entropy H and the values of λ where they are optimal. − indicates absence of known analytical result

Topology	ρ	D	C	H	λ
Poisson	ρ	$\approx \frac{logn}{log(\rho(n-1))}$	ρ	−	0
Star	$2/n$	$\frac{2(n-1)}{n}$	0	$logn - \frac{(n-1)}{n} log(n-1)$	−
Complete	1	1	1	0	1
Linear	$2/n$	$\frac{n+1}{3}$	0	$\frac{1}{n}((n-2)log(n-2) + 2log2) - logn$	$\lambda < 0$

where $D_n(i,j)$ is the minimum distance from the i-th vertex to the j-th vertex. We define the average vertex vertex distance as

$$< D_n >= D_n / \binom{n}{2}$$

If D^k_{n+1} is the contribution to D_{n+1} when the new vertex is linked to the k-th existing vertex, $1 \leq k \leq n$, such an $n+1$-vertex graph obeys

$$D_{n+1} = D_n + D^k_{n+1} \tag{7.6}$$

where

$$D^k_{n+1} = \sum_{i=1}^{k} i + \sum_{i=2}^{n-k+1} i$$

Previous equation leads to

$$D^k_{n+1} = \binom{n+1}{2} \tag{7.7}$$

for $k = 1$ and $k = n$. In general,

$$D^k_{n+1} = k^2 - (n+1)k + \frac{n^2+3n}{2}$$

D^k_{n+1} has one single non-assymptotical minimum (at $k^* = (n-1)/2$) and no non-assymptotical maximum so D^k_n is maximal for $k = 1$ and $k = n$ and $1 \leq k \leq n$. $k = 1$ or $k = n$ correspond to a graph order $n+1$ satisfying (7.2), as we wanted to proof.

Substituting (7.7) into (7.6), we get the longest graph of order n satisfys

$$D_n = D_{n-1} + \binom{n}{2}$$

Expanding the previous recursion we get

$$D_n = \sum_{i=2}^{n} \binom{n}{2} = \frac{1}{2}\left(\sum_{i=1}^{n} i^2 - \sum_{i=1}^{n} i\right)$$

After some algebra we have $D_n = n(n^2-1)/6$ and thus $< D_n >= (n+1)/3$

It can also be shown through induction on n that a star graph with a degree distribution

$$p_k = \frac{n-1}{n}\delta_{k,1} + \frac{1}{n}\delta_{k,n-1} \tag{7.8}$$

has the minimum distance possible among all possible graphs having $n-1$ links. For $n = 2$, the only connected graph (and thus the only with finite distance)

trivially is the best one having $n-1$ links. If we assume that the graph described in (7.8) is the optimal for n vertices, the optimal graph of $n+1$ vertices has $d_{n+1} = d_n + \Delta^k_{n+1}$ where Δ^k_{n+1} is the contribution to D_{n+1} of the new vertex when linked to the k-th existing vertex. Thereafter, $\Delta^1_{n+1} = 2n-1$ and $\Delta^k_{n+1} = 3(n-1)$ for $1 < k \leq n$. $\Delta^1_{n+1} < \Delta^{k>1}_{n+1}$ holds for $n > 2$, so the graph of order $n+1$ obeying (7.8) is also the best one with $n-1$ links.

Acknowledgments

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