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Optimization of spatial complex networks

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HIGHLIGHTS

- Growth model for spatial network subject to optimization criterion.
- Scaling exponent depends on optimization criterion.
- Transition from exponential to scale-free behavior studied.
- Discussion of network size effects.

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ABSTRACT

First, we estimate the connectivity properties of a predefined (fixed node locations) spatial network which optimizes a connectivity functional that balances construction and transportation costs. In this case we obtain a Gaussian distribution for the connectivity. However, when we consider these spatial networks in a growing process, we obtain a power law distribution for the connectivity. If the transportation costs in the functional involve the shortest geometrical path, we obtain a scaling exponent $\gamma = 2.5$. However, if the transportation costs in the functional involve just the shortest path, we obtain $\gamma = 2.2$. Both cases may be useful to analyze in some real networks.

1. Introduction

Complex networks have received substantial attention in recent years, because they provide a useful representation for many technological, biological and social systems [1–4]. Many of the networks in nature have common features, such as the connectivity distribution $P(k)$, which often results to behave as a power law $P(k) \sim k^{-\gamma}$ for large degree k [5–14]. Several authors have developed network models that seek to replicate these distributions. One of the most emblematic cases was proposed by Barabási–Albert [1,15,16], in which a weighted random growth model is used to generate a power law distribution with $\gamma = 3.0$. In this model in each step a new vertex appears and it is connected randomly with a vertex of the network with a probability proportional to its connectivity degree. Empirical networks show similar characteristic exponent γ, such as citation networks [5] and electronic circuits [6]. However there are other important sets of systems which exhibit a network structure with a different exponent, for example: telephone calls [7,8], World Wide Web [9], metabolic [10],

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movie actors [11], protein interaction [12], the internet [13] and word co-occurrence [14]. In these cases, the characteristic exponent γ ranges from 2.0 to 2.7.

Although there are variations to the Barabási–Albert model which generate complex networks with exponents different than 3.0 (*e.g.* mixing of random and preferential attachment, additional attractiveness of nodes, or introducing aging of nodes [1,17]), various authors have proposed models that yield such exponents by considering that the network is subject to a certain optimization process, with respect to a parameter relevant to the network of interest. For example, such models have been considered to describe brain functional networks where the parameter to be optimized is the coherence of coupled oscillators, representing brain regions [18,19]. Discussion of optimized networks leading to scale-free distribution has been made, for instance, in Ref. [20], where trees in software architecture graphs are studied, and optimization is underlying the creation of the graphs by means of the design principles involved in the software creation.

In particular, the role of optimization has been extensively studied in networks where some notion of distance between nodes is relevant. Distance between vertices through the network can be defined as the number of edges necessary to go from one vertex to another. This is important, since it allows to define a distance for arbitrary systems, such as social networks or the World Wide Web, where a physical distance is not necessarily meaningful. However, there is another equally important set of complex networks where vertices do have a definite position in space [21]. We will call them spatial networks, and they are usually related to transportation: city traffic networks, power networks, telephone wiring networks, internet, etc. In all of them, there is some kind of load being carried between vertices, which can be cars in a city traffic network or electricity in power networks. In these spatial networks, the nth vertex is placed at a fixed position (x_n, y_n) in space, and a geometric distance between vertices can be calculated, *e.g.* the Euclidean distance.

Naturally, both distances are in principle completely unrelated: two vertices directly connected by the network could be separated by a very large geometric distance. This leads to an interesting conflict when the evolution of the network is considered: if a new city appears on the map, then what new roads should be built to connect it with the pre-existent cities? The decision could be to connect it with the nearest city, or with the most important one. And, in turn, if the choice is to prioritize connections to a given city, is it better to connect them directly, thus reducing construction costs, or indirectly, passing through some other cities, in order to increase trading between them? It is therefore evident that, in a real evolving transportation network, there arises the issue of how both kinds of distances, geometrical or topological, compete.

Using these spatial networks and these distances, several authors have proposed network models based on some optimization process [22–25]. Regarding transport networks in particular, it seems natural to define two kinds of costs to optimize: the cost of constructing the network and the cost of transporting through it. If someone wants to fabricate an internet network, the cost should be related to the total length of cable that is going to be used, while if somebody wants to elaborate a railway network, the cost should be related to the total length of railroads to be built. Inspired by these examples, we will assume that the cost of constructing a network is proportional to the sum of the length of the connections. On the other hand, the transportation cost is the cost of actually moving the load through the network. For instance, for the railway network, the cost is related to issues such as fuel consumption, wear on the train wheels, etc. Notice that these transportation costs are also related to the length of the connections, but they are not equivalent to construction costs. For instance, it is possible that for a given spatial distribution of cities, building a road between cities A and B would be very expensive, suggesting that it might be better not to spend money building it; however, that road may turn out to improve connectivity in the network as a whole, so that transportation costs end up being attractive. Thus, when assessing the overall cost of a network, the cost of having to build the roads once, and then using them to move load between all the cities, must be considered as two separate contributions to the total cost. In other words, a transport network could be the result of the minimization of some cost function that on the one hand considers the cost of construction, and on the other hand considers the transportation cost. This way of thinking in a transport network has already been developed by some publications at the beginning of the 70s [26,27], and lately it has been widely studied by several authors [28–31].

On this basis, studies of various optimization criteria have been made to determine, for example, how the statistical properties of the resulting complex network acquire small-world or scale-free behavior, and, in the latter case, a range of exponents have been shown to arise. In the case of static networks, where the number of nodes is fixed, optimization can be achieved by rewiring the network, as studied in Refs. [23,32], showing that optimization can lead to small-world and scale-free networks.

Growing networks have also been studied [33–35]. For instance, in computing related networks, such as Ref. [34] where the case of Internet topology was considered, the growth is determined by competition between the cost of connecting a new node and the cost of transmission delays. Optimization of spatial growing networks has also been studied in Ref. [35], where the interplay between the timescales for assembly and for optimization of the network is discussed. Thus, in this case the optimization process involves rewiring of the network after each new node is added to the network, a rewiring which can be either global (new links can involve nodes separated by arbitrary distances) or local (new links are chosen only among nearby nodes). A variety of power-law exponents are shown to emerge.

In this work, we intend to study the effect of different optimization criteria on the degree distribution of spatial networks. In Section 2 a Global Optimization Model is discussed, where all vertices are initially known, and edges are created according to a certain optimization criterion. Then, Sections 3 and 4 deal with a Weighted Growth Optimization Model, where at each step a new vertex appears and it is then connected with a vertex of the network, again following an optimization criterion. In Section 5, a more detailed analysis of the dependence of the resulting networks on the relative weight of costs, along with a discussion of size effects, is carried out. Finally, in Section 6 results are summarized and discussed.

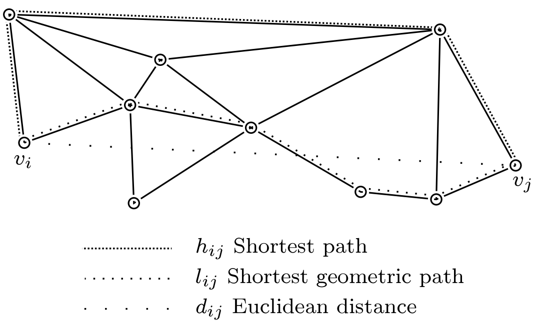

Fig. 1. Comparison between the distances d_{ij}, l_{ij} and h_{ij}, for vertices v_i and v_j in a network.

2. Global optimization model

In this case, we are interested in a spatial network where the location of all vertices is known from the start, and the problem is to find the set of "optimal" edges to connect them.

As mentioned above, several definitions of distance are possible. We will consider three of them, illustrated in Fig. 1 for two vertices v_i and v_j. d_{ij} is the Euclidean distance between the vertices, and is the shortest distance between them when regarded as points on the plane; l_{ij} is the shortest geometrical path, and is the shortest length between the vertices when traveling along the network; finally, h_{ij} is the shortest path, and is the minimum number of edges which have to be traveled to go from one vertex to the other. Notice that d_{ij} and l_{ij} are different in general, unless the vertices are connected by edges which form a single straight line.

Gastner and Newman [28–30] have discussed various transport network models based on optimization. In particular, we are interested in one where there are two costs associated with the existence of the network: the cost of construction of the network, and the cost of load transportation over the network.

The construction cost is related to actually building each edge, so in our model we consider that it is given by the sum of all lengths of the connections between vertices:

$$D = \sum_{i<j} A_{ij} d_{ij}, \tag{1}$$

where d_{ij} is the Euclidean distance between vertices v_i and v_j, and A_{ij} the adjacency matrix ($A_{ij} = 1$ if vertices i and j are connected, and $A_{ij} = 0$ otherwise).

On the other hand, the transportation cost is related to actually traveling along the network, to move load between any two given vertices. If load has to be moved from a vertex v_i to a vertex v_j, and assuming that we intend to minimize costs, then we may regard the transportation cost for this load as the length of the shortest geometrical path l_{ij} between both vertices. Therefore, when all possible pairs of vertices are considered, the transportation cost for the complete network can be estimated as

$$L = \sum_{i<j} l_{ij}, \tag{2}$$

which can also be found in terms of the adjacency matrix A_{ij} and the Euclidean distance matrix d_{ij}.

Finally the cost of the network can be written as

$$E(\lambda) = (1 - \lambda)D + \lambda L, \tag{3}$$

where λ is a real number ($0 < \lambda < 1$) which measures the relative importance of construction versus transportation costs. Then, for a given value of λ, $E(\lambda)$ should be minimized as a function of the edge configuration (that is, the adjacency matrix $\mathbf{A}$).

Notice that, in general, the construction and transportation costs could be proportional to D and L, say αD and βL, respectively. These parameters would increase or decrease the relative importance of D and L, besides the effect of λ. In Eq. (3), however, we state that the relative importance depends only on λ, which linearly interpolates the cost between D and L.

As mentioned above, for this model the number and location of the vertices is initially known. They are taken from a homogeneous random distribution of points on a plane. Then, the optimal set of edges is found. To find the minimum of Eq. (3) it is necessary to calculate all possible configurations of A ($2^{[\frac{1}{2}N(N-1)]}$ combinations) which is computationally very expensive. For this reason, an alternative method was used to find an approximate minimum.

The method employed was the same that was used by Gastner and Newman, [29] which uses the Ramalingam–Reps algorithm [36]. The method is as follows. We start with a random configuration of edges, and at every step we take two

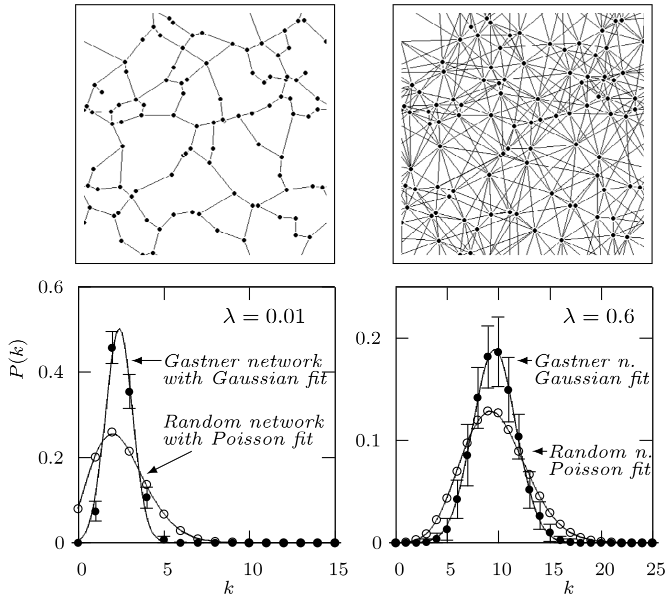

Fig. 2. Networks obtained by minimizing Eq. (3), for $N = 100$ vertices, and for two values of λ. In the lower panel, is shown the distribution of connectivity of each network, averaged over an ensemble of 50 different spatial configurations and fitted by a Gaussian distribution. Additionally for each case is shown the distribution of the respective random network (with same number of vertices and edges).

random vertices v_i and v_j. If these are connected we eliminate the edge ($A_{ij} = 1 \rightarrow A_{ij} = 0$) with probability

$$P = \begin{cases} 1 & \text{if } E_{\text{new}} < E_{\text{old}} \\ \exp\left[-\frac{1}{T}(E_{\text{new}} - E_{\text{old}})\right] & \text{otherwise,} \end{cases}$$

where E_{old} is the value of Eq. (3) before deleting the edge and E_{new} is the value of Eq. (3) after removing it. If the vertices v_i and v_j are not connected we connect them ($A_{ij} = 0 \rightarrow A_{ij} = 1$) with the same probability, but this time E_{old} is the value of Eq. (3) without the new edge and E_{new} is the value with the new edge.

In the equation, T is a constant related to the "temperature of the system" which initially has a value of $T = 10$. The minimization is as follows: for a fixed value of T we take each pair of vertices in the network in random order and we eliminate or create edges with a probability P. Then, we decrease the value of T by a factor 0.9 ($T_n = 0.9 \cdot T_{n-1}$) and again we take each pair of vertices in random order and we eliminate or create edges with a probability P. We repeated this process for each "temperature" until $T = 10^{-5}$, where there is very low probability that there is a change.

Fig. 2 shows some results of the model simulations made for different values of λ. It can be seen that the connectivity distributions follow a Gaussian curve. This result is similar to the random networks, which follow Poisson distributions [1–4]. This is interesting since, as discussed in Section 1, real networks are typically scale-free. In order to address this, a variation of this model is presented in Section 3, where the network is the result of an optimized growth process, and distributions more consistent with real networks can be obtained.

3. Weighted Growth Optimization Model

The previous model assumes that the position of the vertices on the plane is known since the beginning. This contrasts with a large number of real cases where the formation of the network is the result of a dynamic process of growth, and the location of future vertices is not known. For instance, in a region where there are already cities and roads, a new city may appear which needs to be connected to the rest; or a new station is added to a pre-existent railway network. In order to take into account this dynamics, we propose here a model that incorporates this notion of growth, while maintaining the notion of efficiency described in Section 2.

The model begins with a single vertex v_0. Then, a new vertex v_1 appears at some random position in the plane. Vertex v_1 can only be connected to vertex v_0 as it is the only one in the plane. The next vertex, v_2, must choose to which of the existing vertices in the network to connect. In order to keep the model simple, when a new vertex appears, it connects to a single pre-existent vertex. These choices determine the final geometry of the network. In the model of Barabási [15] the new vertex connects with a previous vertex with probability proportional to the degree of connectivity of the existing vertices, which provides a measure of "popularity" of the vertices. This leads to scale-free networks, with scaling exponent equal to 3. In our model, we propose that each new vertex v_n must connect to vertex v_m such that the cost function of the network, given in Eq. (3), is minimized.

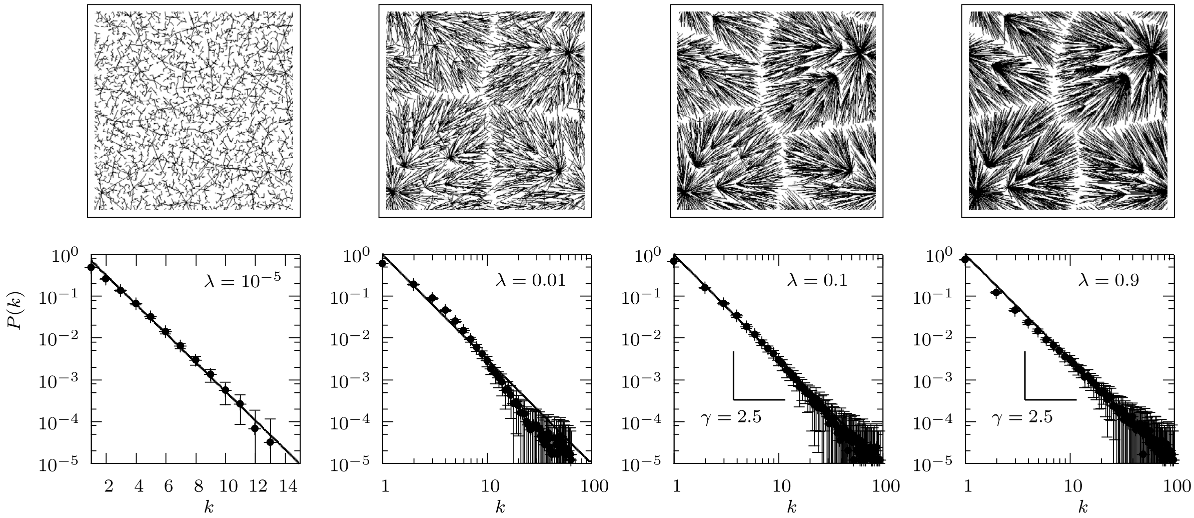

Fig. 3. Results of the simulations of the growing network, as described in Section 3, using Eq. (4) for different values of λ. Upper panel: networks obtained from the growth process, all of them using the same spatial configuration of vertices, in order to highlight the effect of λ. Lower panel: distribution of connectivity, calculated over an average on 50 spatial configurations, each one with $N = 5000$ vertices. We note that for values of λ close to zero the distribution follows a negative exponential, while for higher values the distribution follows a power law for large k.

Because the location of future vertices is not known, the optimization criterion can only take into account the current state of the network. Thus, since all edges are permanent once created, it is expected that the resulting network may be very different to the ones obtained in Section 2, where even though the optimization function is the same, decisions are taken while knowing the location of all vertices.

Once a new vertex v_n appears its position is fixed in the plane, with the only remaining variable being the edge location. Given Eq. (3), the cost increment due to this new edge is

$$\Delta E(\lambda) = \min_m \left((1-\lambda) d_{nm} + \lambda \sum_{i=0}^{n} l_{ni}(m) \right), \tag{4}$$

where d_{nm} is the Euclidean distance between v_n and v_m, and $l_{ni}(m)$ is the shortest geometric path between v_n and v_i, given that v_n is connected to v_m. The minimum is found by simply considering each pre-existing node m, calculating the cost function by connecting to this mth node, and then the node which yields the lowest cost function is chosen. Notice that, at each step, in order to minimize $\Delta E(\lambda)$, each new vertex v_n is connected to a vertex v_m that must be both near (low value of d_{nm}) and at a "privileged position" in the network, that is, with high accessibility to all other vertices in the network (low value of $\sum_i l_{ni}(m)$). The latter is, to some extent, similar to the "popular" notion put forward by Barabási [15], and we could expect that, if λ is large enough, this model will lead to scale-free networks.

On the other hand, if λ is small, the cost function is dominated by the Euclidean distance between nodes. But this term depends on the random spatial position of the nodes, and thus the optimization process is equivalent to a random choice of edges. Therefore, an exponential decay is expected in this case.

Fig. 3 shows results of the simulation model for different values of λ. Connectivity distributions correspond to an average over 50 different runs (which yield 50 different spatial configurations, each one with $N = 5000$ vertices). We note that for $\lambda \approx 0$ the vertices are connected with the nearest vertex, leading to a connectivity distribution which is a negative exponential. As expected, for slightly larger values of λ the vertices seek to connect with "popular" vertices, leading to power law distributions, which is also expected. However, what is interesting in this case is that the characteristic exponent is $\gamma = 2.5$, which fits many real networks, and is clearly different from the Barabási result, $\gamma = 3$ [15].

Certainly, various values of γ can be obtained for spatial networks, either static or evolving, by using different growth algorithms, optimization strategies, and cost functions [23,32–34]. In Ref. [35], for instance, a detailed analysis of the process is made, by considering optimization with respect to the average path length on the network (our l_{nm}, essentially), and showing the effect of the ratio of timescales for assembly and optimization of the network τ; and also on the locality of the optimization process, and its effect on the topological structure of the network. Our case, where optimization is carried out every time a new node is added, would correspond to the regime $\tau = 1$, where assembly and optimization fully compete. In our work, though, optimization is not done via rewiring, which is typically not an option for road networks. However, it is worth noting that, as suggested in a number of references, *e.g.* in Refs. [34,35], in our model the scale-free features arise from the competition of various constraints on the network growth, but they are nevertheless a robust behavior present on a relatively large fraction of parameter space.

Fig. 3 displays results for a few specific values of λ. Later, in Section 5, we will study in more detail the evolution of the network as a function of λ.

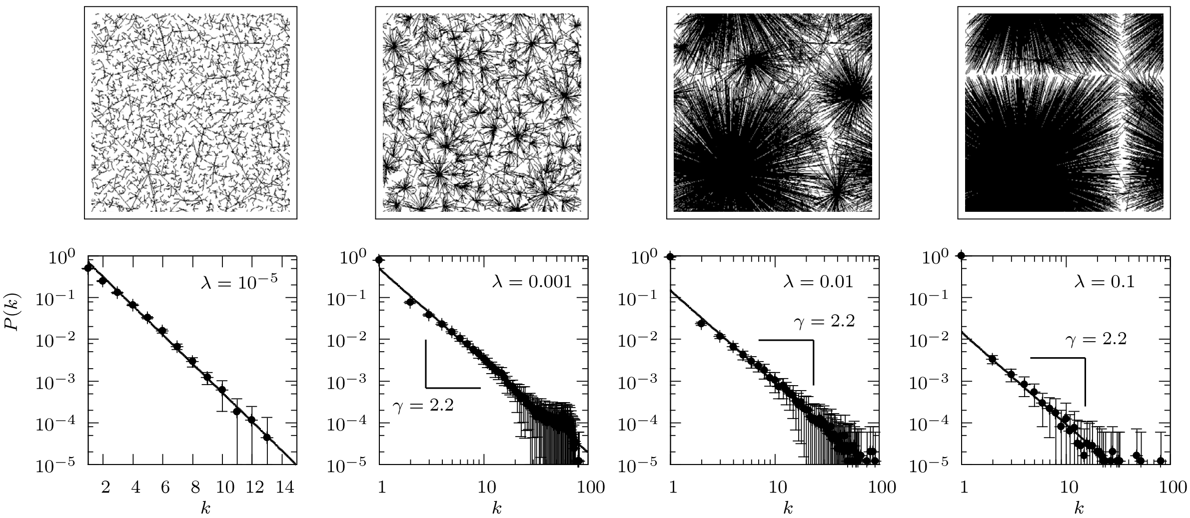

Fig. 4. Results of the simulations of the growing network, as described in Section 4, using Eq. (5) for different values of λ. Upper panel: networks obtained from the growth process, all of them using the same spatial configuration of vertices, in order to highlight the effect of λ. Lower panel: distribution of connectivity, calculated over an average on 50 spatial configuration, each one with $N = 5000$ vertices. We note that for values of λ close to zero the distribution follows a negative exponential, while for higher values the distributions follow a power law for large *k*.

4. And if we slightly change the cost function?

For some real networks the cost function given by Eq. (3) may not be representative. For example, for a network of buses the number of stops may be more important than the path length. Following this idea, some authors propose functions including the cost of the shortest paths instead of the shortest geometric path [23,25,28–30]. In that case, instead of Eq. (4), the cost increment due to a new vertex is

$$\Delta E(\lambda) = \min_m \left((1-\lambda) d_{nm} + \lambda \frac{1}{\sqrt{N}} \sum_{i=0}^{n} h_{ni}(m) \right), \quad (5)$$

where d_{nm} is the Euclidean distance between v_n and v_m, and $h_{ni}(m)$ is the shortest path between v_n and v_i, given that v_n is connected to v_m. The term $1/\sqrt{N}$ is just a scale factor. It is added because d_{ij} and h_{ij} are quantities of different orders. For instance, if we consider (as we have in this paper) vertices in a square of side equal to 1, then if we distribute N vertices uniformly in the square, for N large enough, then the typical distance between vertices is $d \simeq 1/\sqrt{N}$. However, the shortest geometrical path between them is, if they are connected, $h \simeq 1$, which is much larger than d. Therefore in Eq. (5), the contribution of the second term would be dominant for most values of λ. Thus, we add this $1/\sqrt{N}$ scale factor so that the dominant effect on the competition of both distances is the interpolating factor λ. Fig. 4 shows results of the simulation model for different values of λ. Connectivity distributions correspond to an average over 50 different runs (which yield 50 different spatial configurations, each one with $N = 5000$ vertices).

The behavior is qualitatively similar to the previous case: connectivity distributions which are best fitted by negative exponentials for $\lambda \approx 0$, and by power laws for larger values of λ. These limits can be understood in the same way as discussed in Section 3. However, it is found that the characteristic exponent is $\gamma = 2.2$, which is also in the correct range for real networks, but is different to the results in Section 3.

This is interesting, because it is expected that real networks are in general the result of an evolutionary process, and our findings show that growth following an optimization criterion leads in general to scale-free networks, as those observed in nature. But not only that: our results also suggest that the variety of scaling exponents found in nature could be explained by different underlying optimization processes.

5. Network dependence on λ

As mentioned above, Figs. 3 and 4 display results for a few values of λ. One can better appreciate the transition from exponential to power-law behavior by estimating the extent to which the observed distribution (for all values of *k*) can be actually fitted by either model. Thus, a least square fit of an exponential distribution for the case $\lambda = 10^{-5}$ in Fig. 3 or Fig. 4 should yield a small error, whereas a power-law distribution should yield a large error; the opposite should occur for the case $\lambda = 0.9$. Specifically, we can estimate the error in the exponential or power-law fit as the relative error in the slope of the semilog or log–log fit, respectively. Fig. 5 shows the fitted error in the slope for both distributions as a function of λ. We have considered the case of the cost function given by Eq. (5), as shown in Fig. 4, but results for Eq. (4) are similar.

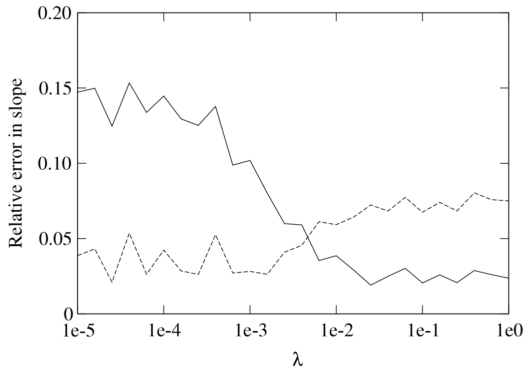

Fig. 5. Relative error for the slope in a semilog plot (dashed line) and a log–log plot (solid line) for the degree distributions in Fig. 3, obtained by local optimization of a network with $N = 1000$ vertices, and several values of λ. The crossing of both lines yields an estimation of the transition point from an exponential distribution to a power-law one.

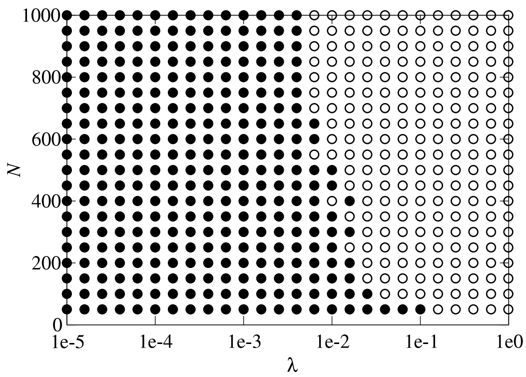

Fig. 6. Phase space for exponential/scale-free behavior, as a function of λ and network size N. Filled circles mark zones where exponential behavior better fits the degree distribution; open circles, where scale-free behavior dominates.

It is observed that, in effect, the exponential fit is better for very small values of λ, whereas the power-law fit is better for larger values. The plot also allows us to estimate the transition point between both regimes, which turns out to be around $\lambda \simeq 0.004$.

This being a growing network, it is also interesting to investigate how the exponential/scale-free behavior evolves as the system size increases. We study this by estimating the transition value of λ between both regimes, as in Fig. 5, but for several values of N. Results are shown in Fig. 6. It is observed that, as network size increases, the transition to scale-free behavior occurs for lower values of λ. However, this trend saturates at about $N = 700$, as can be seen in Fig. 6.

It can also be observed that, due to the optimization process, the total Euclidean distance D between nodes in the network behaves differently to their distances along the network. One of these distances is the sum of the shortest geometric paths along the network, as defined in Eq. (2). Similarly, and following Fig. 1 and Eq. (5), we can define a total distance based on the shortest path along the network:

$$H = \sum_{i<j} h_{ij}. \tag{6}$$

In Fig. 7 we show the evolution of these three distances, D, L, and H, as a function of λ, for two network sizes: $N = 50$ and $N = 1000$.

It can be observed that the optimization process leads to a similar trend for both distances along the network: H, which only takes into account the number of edges that connect any two nodes; and L, which considers the physical length of those edges. This is interesting, as the optimization was on the cost function Eq. (4), which should naturally affect L. However, decreasing the length of the road between two nodes is similar to decreasing the number of roads between them (consider that nodes are chosen within a given square region, which could lead to arbitrarily large values of l_{ij}, maintaining low values of h_{ij}), and thus H follows a similar trend as L.

On the other hand, D follows the opposite trend, as it increases with λ, which is a manifestation of the competition between D and L as expressed in the cost functions Eqs. (4) and (5).

These trends for L and H do not change with N, as can be seen in Fig. 7, where $N = 50$ and $N = 1000$ (the minimum and maximum values used in Fig. 6 are shown). The curves for the intermediate values of N fill the space between the two curves shown in Fig. 7, and have not been shown for simplicity.

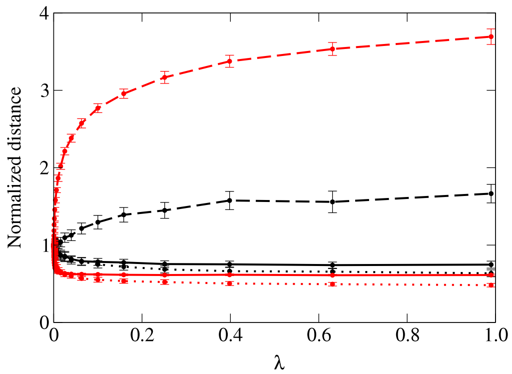

Fig. 7. (Color online) Distances in the network, D (dashed lines), L (solid lines), H (dotted lines), as a function of λ. Points correspond to an average over 50 runs, and error bars to the corresponding standard deviation of the data. All values are normalized to the respective distances for the minimum value of λ (10^{-5}). Two network sizes are considered, $N = 50$ (black lines) and $N = 1000$ (red lines).

Also notice that although trends do not change, the various distances are sensitive to different degrees on N. As shown in Fig. 7, distances along the network (L and H) weakly depend on N, whereas the Euclidean distance between nodes (D) clearly increases with N. This is expected since our growth model positions the location of new nodes randomly, and later chooses its connections by an optimization algorithm. As a consequence, adding a node has the obvious effect to increase the total distance between all possible pairs of nodes, whereas L and H are constrained by optimization, with already fixed nodes locations.

6. Summary

We have studied the creation of complex spatial networks that are built using an optimization criterion. We studied two scenarios: (a) the connection of a fixed set of vertices with initially known locations, and (b) a growing network in which every new vertex must be connected to a pre-existent one. The optimization must balance between the cost of building the edges (related to the Euclidean distance between vertices) and the cost of transporting over the network (related with the shortest paths between the vertices).

When all vertices are fixed at known locations before constructing the network, the optimization process successfully yields networks with a Poisson distribution of connectivity. As for the growing network, the optimization model leads to scale-free distributions with characteristic exponents $\gamma = 2.5$ and $\gamma = 2.2$ when the cost function includes the shortest geometric path and shortest path, respectively. It is interesting to note that the same scalings are found in some real networks [37–39].

We believe that the very simple network optimization model described here can provide insight into the evolution of some real networks that involve transport of things, such as roads, the Internet, or electric networks.

Acknowledgments

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