Self-similarity of complex networks and hidden metric spaces

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We demonstrate that the self-similarity of some scale-free networks with respect to a simple degree-thresholding renormalization scheme finds a natural interpretation in the assumption that network nodes exist in hidden metric spaces. Clustering, i.e., cycles of length three, plays a crucial role in this framework as a topological reflection of the triangle inequality in the hidden geometry. We prove that a class of hidden variable models with underlying metric spaces are able to accurately reproduce the self-similarity properties that we measured in the real networks. Our findings indicate that hidden geometries underlying these real networks are a plausible explanation for their observed topologies and, in particular, for their self-similarity with respect to the degree-based renormalization.

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Self-similarity and scale invariance are traditionally known as characteristics of certain geometric objects, such as fractals [1], or of field theories describing system dynamics near critical points of phase transitions [2]. In these cases, objects or physical systems are intrinsically embedded in metric spaces and distance scales in these spaces are natural scaling factors. In complex networks [3], scale invariance is traditionally restricted to the scale-free property of the distributions of node degrees, which in a vast majority of complex networks follow power laws of the form \( P(k) \sim k^{-\gamma}, \gamma \in [2,3] \). In search for more complete self-similar descriptions, several recent works [4] introduced box-covering renormalization procedures, applied them to a few real networks, and found that certain networks, e.g., the Web and some biological networks, have finite fractal dimensions and degree distributions that remain invariant.

Despite this promising progress, self-similarity and scale invariance of complex networks are still not well defined in a proper geometric sense. The reason is that many complex networks are not explicitly embedded in any physical space. As such, they lack any metric structure, except the one that their graph abstractions induce by the collection of lengths of shortest paths between nodes. However, this observable topological metric is a poor source of length-based scaling factors. It does not have large lengths as it exhibits the small-world [5] or even ultrasmall-world [6] property, meaning that the characteristic path lengths grow not polynomially but (sub)logarithmically with the network size. The apparent absence of any other metric structures supports the common belief that complex networks cannot be invariant under geometric length scale transformations.

In this paper, we undermine this belief by introducing the concept of hidden metric spaces as natural reservoirs of distance scales with respect to which scale-free networks may be self-similar at all scales. At the formal level, hidden metric spaces are variations of hidden variables [7,8,9]. Specifically, we assume that all network nodes, in addition to forming an observed network topology, reside in an underlying hidden metric space, meaning that for all pairs there are defined hidden distances satisfying the triangle inequality, which can be arbitrarily large. If hidden metric spaces do exist and play a role in shaping the observed network topologies, then strong clustering—the high concentration of triangles—arises as a natural consequence of the triangle inequality in the underlying geometry. Therefore, we focus on clustering as a potential connection between the observed topologies and hidden geometries.

Consider the following degree-thresholding renormalization procedure, which produces a hierarchy of subgraphs within a given graph \( G \) as illustrated in Fig. 1. For each degree threshold \( k_T = 0,1,2,\ldots \), first extract from \( G \) the subgraph \( G(k_T) \) induced by nodes with degrees \( k > k_T \). Second, for each node in \( G(k_T) \), compute its internal degree \( k_i \), i.e., the number of links that connect a given node to other nodes in \( G(k_T) \) and, finally, rescale \( k_i \)'s by the average internal degree \( \langle k_i \rangle(k_T) \) in \( G(k_T) \) to obtain the rescaled quantity \( k_i / \langle k_i \rangle(k_T) \).

We applied this procedure to a few real complex networks and found that their main topological characteristics—degree distributions, degree-degree correlations, and clustering—are self-similar with respect to the described procedure: both before and after renormalization with different values of threshold \( k_T \), all these characteristics closely follow the same master curves describing the topological structure of the whole subgraph hierarchy. We next randomized the observed topologies preserving the degree distribution as in [10], and found that their degree distributions and degree-degree correlations are still self-similar, but clustering is not.

We provide examples of these empirical observations in Fig. 2 where we show the degree-dependent clustering
The coefficient of the renormalized graphs $G(k_T)$ with different $k_T$’s for the real and randomized topologies of the Border Gateway Protocol (BGP) map of the Internet at the Autonomous System level [11] and of the Pretty Good Privacy (PGP) social web of trust [12]. Both the BGP and the PGP are scale-free networks with exponents $\gamma_{BGP} = 2.2 \pm 0.2$ and $\gamma_{PGP} = 2.5 \pm 0.2$. For brevity, we omit plots showing self-similarity of degree distributions and degree-degree correlations. Fig. 2 shows that even though the internal average degree $(k_i(k_T))$ grows significantly for all networks, the average clustering coefficient of $G(k_T)$ as a function of $k_T$, $c(k_T)$, is nearly constant for the subgraphs of the real topologies, but it grows for their randomized counterparts. We also experimented with airport networks [13] and found that they exhibit qualitatively the same results as the Internet (BGP) and the social (PGP) networks. The BGP and PGP networks are more interesting and challenging for our purposes since, as opposed to airport networks, they appear to be not explicitly embedded in any observable physical space.

The high levels of clustering observed in real networks and their self-similarity under the degree thresholding renormalization find a plausible explanation in the assumption that some metric structures underlay the observed network topologies. Indeed, under this assumption, clustering becomes a natural consequence of the triangle inequality in the metric space underneath. The fact that the randomized networks are not self-similar (cf. Fig. 2 b,d) also supports this observation. The applied degree-preserving randomization is a process that involves pairs of nodes, whereas the triangle inequality concerns node triplets. Therefore, this randomization process cannot fully preserve the network properties imposed by the triangle inequality.

In the rest of the paper, we provide further evidence that this metric space explanation is indeed plausible. We do so by introducing a class of network models designed with the following three objectives: we want all nodes to exist in a metric space underlying the network topology; we want to control the degree distribution and clustering, so that we can generate scale-free graphs with strong clustering; and we want these graphs be small-world. We then find that the networks generated by our model reproduce all the self-similar effects that we have empirically observed in real networks. We emphasize that although there are models of scale-free networks embedded in Euclidean lattices [14], none can simultaneously reproduce all the effects discussed above.

To define our model, we use the hidden variables formalism [15] taking as hidden variables nodes’ coordinates in a metric space. Each two nodes are located at a certain distance $d_{ij}$, which relates the network topology to the underlying metric space. This probability depends on the metric distance $d = r(d/d_c)$, where $d_c$ is the characteristic distance scale, i.e., a parameter that calibrates whether a given distance is short or long. Function $r$ must be a positive integrable function of $d \in [0, \infty)$. Consequently, nodes that are close to each other in the metric space are more likely to be connected in the graph.

To engineer full control over the degree distribution, we link the characteristic distance scale $d_c$ to the topology of the network. We assume that $d_c$ is not a constant but depends on some topological properties of the nodes. Specifically, we assign an additional hidden random variable $\kappa$ to each node, which corresponds to its expected degree. For simplicity, let our hidden metric space be a homogeneous and isotropic $D$-dimensional space. Then the choice guarantees that the average degree of nodes with variable $\kappa$ is $\bar{\kappa}(\kappa) = \kappa$. Therefore, the distribution $\rho(\kappa)$ of this variable is asymptotically equal to the degree distribution $P(k)$ in the resulting networks [7].

Eq. (1) has another important consequence: high degree nodes –hubs– are likely to be connected regardless their distance in the metric space because $d_{ij}(\text{hub,hub})$ is large. Low degree nodes, on the other hand, are connected only if they are close, whereas hubs are connected to low degree nodes if their distances are at most intermediate. This pattern is typical of real networks embedded in metric spaces, such as the airport network. It is very likely that two major hubs like New York and London are connected, but it is very unlikely that two small airports are connected, unless they are close enough.

We can now generate graphs with any degree distribution by choosing an appropriate $\rho(\kappa)$. In particular, to generate scale-free graphs we set $\rho(\kappa) = (\gamma - 1)\kappa^{-\gamma} \kappa^{\gamma - 1}$, $\kappa > \kappa_0 \equiv (\gamma - 2)/(\gamma - 1)$, $\gamma > 2$, which after transformations described in [12] yields the degree distribution

$$P(k) = (\gamma - 1)\kappa_0^{\gamma - 1}\Gamma((k + 1 - \gamma)\kappa_0)/k!,$$

where $\Gamma$ is the incomplete gamma function. The asymptotic behavior of this degree distribution for large $k$ is $P(k) \sim k^{-\gamma}$, i.e., the same as of $\rho(\kappa)$. This result is independent of the dimension of the hidden metric space and it is valid for any integrable connection probability of the form $r(d/d_c)$, where $d_c \equiv d_c(\kappa, \kappa')$ is any function that factorizes in terms of $\kappa$ and $\kappa'$. 

![FIG. 1: Sketch of the degree-thresholding renormalization.](image_url)
where $d$ the more triangles are formed. The exact dependence of $\alpha$ function of the rescaled internal degree for the Internet BGP map, the PGP web of trust, and their randomized versions. $\omega$: Average clustering coefficient as a function of the threshold degree $k_T$ for renormalized real networks and their randomized counterparts. $\omega$: Internal average degree as a function of $k_T$ for the same networks.

Given the freedom in the choice of the space dimension and particular form of $r$, we hereafter consider the simplest one-dimensional model. We place nodes on a circle, $\mathbb{S}^1$, by assigning them a random variable $\theta$ representing their polar angle uniformly distributed in the interval $[0, 2\pi)$. The circle radius $R$ grows linearly with the total number of nodes $N$, $2\pi R = N/\delta$, in order to keep the average density of nodes on the circle fixed to a constant value $\delta$ that, without loss of generality, we set to $\delta = 1$. We specify the connection probability $r$ such that we can control clustering in the generated graphs. Specifically, we define $r$, compliant with Eq. (1), as

$$r(\theta, \kappa; \theta', \kappa') = \left(1 + \frac{d(\theta, \theta')}{\mu R^2}\right)^{-\alpha}, \quad \alpha > 1,$$

where $d(\theta, \theta')$ is the geodesic distance over the circle, i.e., the metric distance $d$ between nodes discussed above, and $\mu = \frac{\alpha - 1}{2(k)}$ is given by the normalization condition $\langle k \rangle = N/(2\pi)^2 \int \rho(\kappa)\rho(\theta, \kappa; \theta', \kappa')\rho(\kappa')d\theta d\theta' d\kappa'$ for large $N$. Parameter $\alpha$ controls clustering. The larger $\alpha$, the more preferred short-distance connections; thus, the more triangles are formed. The exact dependence of the average clustering $\bar{c}$ on $\alpha$ is not important, but both our analytic and simulation results confirm that, as expected, $\bar{c} \to 0$ when $\alpha \to 1$, and that $\bar{c}$ converges to a constant value, dependent on $\gamma$, when $\alpha \to \infty$. We skip the details for brevity; they will be published elsewhere.

We next check whether our synthetic graphs are small worlds, as spatially embedded networks do not always have this property [14, 16]. To this end, we compute the probability $p(d, \kappa|\kappa')$ that a node with hidden variable $\kappa'$ has a neighbor with hidden variable $\kappa$ at geodesic distance $d$ on $\mathbb{S}^1$. We use the hidden variables formalism [7] and the result reads

$$p(d, \kappa|\kappa') = \frac{2}{\kappa^2} \rho(\kappa) \left(1 + \frac{d}{\mu R^2}\right)^{-\alpha}.$$

Integration over $\kappa$ gives the probability that a node has a neighbor at distance $d$. For large $d$, this function scales as $p(d|\kappa') \sim d^{-\alpha}$ when $\alpha < \gamma - 1$ and $p(d|\kappa') \sim d^{1-\gamma}$ when $\alpha > \gamma - 1$. The network is a small world when the average hidden distance to nearest neighbors $\bar{d}(\kappa') = \int x p(x|\kappa')dx$ diverges in the large-$N$ and, consequently, large-$R$ limit. Such divergence indicates the presence of links connecting nodes located at all, including arbitrarily large, hidden distance scales. This average distance $\bar{d}(\kappa')$ diverges when the exponent of the asymptotic form of $p(d|\kappa')$ for large $d$ is smaller than 2, i.e., when either $1 < \alpha < 2$ or $2 < \gamma < 3$, or both. Real scale-free networks have values of $\gamma$ between 2 and 3, meaning that they correspond to the class of small-world networks in our model, regardless of the value of $\alpha$.

Finally, we analyze the self-similarity of networks produced by our model. Thanks to the proportionality between $\bar{k}(\kappa)$ and $\kappa$, we can work in the $\kappa$-space instead of the $k$-space. Since $\rho(\kappa)$ is a power law, the distribution of $\kappa$ for nodes in the subgraph $G(\kappa_T)$ (with $\kappa > \kappa_T$), $\rho(\kappa|\kappa_T)$, is given by the same power-law function but
starting at $\kappa_T$ instead of $\kappa_0$. Therefore, the average of $\kappa$ within $G(\kappa_T)$ is given by $\langle k/\kappa_T \rangle = \langle k \rangle / \kappa_T$. The number of nodes in $G(\kappa_T)$ is $N\kappa_T^{1-\gamma}$, so that their density in $\mathbb{S}^1$ is $\delta(\kappa_T) = \delta \kappa_T^{1-\gamma}$, where $\delta$ is the density of the original graph $G$. Since the connection probability does not depend on $\kappa_T$, subgraphs $G(\delta)$ are replicas of $G$ after the following renormalization of the parameters:

$$\kappa_0 \to \kappa_T \quad ; \quad \delta \to \delta \kappa_T^{1-\gamma}.$$  \hfill (5)

In particular, the average degree of nodes with hidden variable $\kappa$ in $G(\kappa_T)$, $\bar{k}_i(\kappa_T)$, and the average degree of all nodes in $G(\kappa_T)$, $\langle k_i(\kappa_T) \rangle$, are

$$\bar{k}_i(\kappa_T) = \kappa_T^{3-\gamma} \kappa$$

and $\langle k_i(\kappa_T) \rangle = \kappa_T^{3-\gamma} \langle k \rangle$.  \hfill (6)

The degree distribution in $G(\kappa_T)$ is given by the same analytic expression Eq. (2), except that $\langle k_i(\kappa_T) \rangle$ from Eq. (6) replaces $\langle k \rangle$ in Eq. (2).

The exact expression for clustering in $G(\kappa_T)$ is rather long and we omit it here for brevity, but it can be easily derived from results in [7]. What matters for our analysis is that the clustering coefficient of nodes with hidden variable $\kappa$ in $G(\kappa_T)$ satisfies $\bar{c}(\kappa_T) = f(\kappa/\kappa_T)$, where $f$ is some function. It follows that the average clustering coefficient in $G(\kappa_T)$, $\bar{c}(\kappa_T) = \int_{\kappa_T} d\kappa \rho(\kappa) \bar{c}(\kappa_T) = \bar{c}(\kappa_T)$, takes a finite value independent of $\kappa_T$. Using once again the proportionality between the $\kappa$-space and $k$-space and the scaling relations in Eq. (6), we conclude that

$$\bar{c}(k|\kappa_T) \approx f(\kappa/k_T^{3-\gamma}) = \bar{f}(\kappa/k_T^{3-\gamma}),$$

where we use the symbol “$\approx$” to account for fluctuations of degrees of nodes with small values of $\kappa$.

In Fig. 3 we show that our simulation results match perfectly the scaling of clustering predicted by Eq. (7). The same figure demonstrates that the clustering-related self-similarity properties of our modeled networks and their randomizations are qualitatively the same as of real networks in Fig. 2. We emphasize that the self-similarity of clustering observed in our model does not depend either on the dimension of the hidden space or on the final form of $r$. The only requirements are that nodes are located in a metric space and connected under the integrable connection probability $r(d/d_c)$ with $d_c$ given by Eq. (1), and that the degree distribution is scale-free.

In summary, hidden geometries underlying the observed topologies of some complex networks appear to provide a simple and natural explanation of their degree-renormalization self-similarity. If we take the most generic interpretation of hidden distances as measures of either structural or functional similarity between nodes [17,27], and admit that more similar nodes are more likely to be connected, then the hidden and observable forms of transitivity become clearly related. At the hidden geometry layer, this transitivity is the transitivity of “being close,” while at the observed topology layer, it is the transitivity of “being connected.” In future work, hidden metric spaces may find far-reaching applications such as the design of efficient routing and searching algorithms for communication and social networks. Also worth pursuing is studying the relationship between fractality in [4] and self-similarity under our renormalization procedure.

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[18] In the BGP network, nodes are Autonomous Systems that may consist of a large number of routers spreading countries and even continents. Therefore, the physical geography plays only a mild role in the network formation.