On Hypercomplex Networks

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The concept of ‘complexity’ plays a central role in complex network science. Traditionally, this term has been taken to express heterogeneity of the node degrees of a therefore complex network. However, given that the degree distribution is not enough to provide an invertible representation of a given network, additional complementary measurements of its topology are required in order to complement its characterization. In the present work, we aim at obtaining a new model of complex networks, called hypercomplex networks – HC, that are characterized by heterogeneity not only of the degree distribution, but also of a relatively complete set of complementary topological measurements including node degree, shortest path length, clustering coefficient, betweenness centrality, matching index, Laplacian eigenvalue and hierarchical node degree. The proposed model starts with uniformly random networks, namely Erdős-Rényi structures, and then applies optimization so as to increase an index of the overall complexity of the networks. An optimization approach has been considered in terms of gradient descent. The complexity index expresses the dispersion of the several considered measurements. Several interesting results are reported and discussed, including the fact that the HC networks define, as the optimization proceeds, a trajectory in the principal component space of the measurements that tends to depart from the considered theoretical models (Erdős-Rényi, Barabási-Albert, Waxman, Random Geometric Graph and Watts-Strogatz), heading to a previously empty space (low density of cases). We observed that, after a considerably large number of optimization steps, peripheral branching tends to appear that further enhances the complexity of these networks.

I. INTRODUCTION

Network science has progressed a long way from its beginnings in about 2000, to the extent of becoming one of the most popular and widely applied areas in modern science (e.g. [1]). To a good extent, the importance of network science derives from two main facts: (i) being graphs, complex networks correspond to one of the most general discrete structures – encompassing trees, lattices – therefore allowing effective representation of any discrete system or problem; and (ii) the basic idea of complex network is accessible even to non-experts, allowing it to be understood and applied in a wide inter- and multidisciplinary manner.

Yet, despite the intrinsic simplicity of the idea of graph, the concept of complex networks remains a challenge to be conceptually understood. The main issue here regards the term complex. The most typically taken interpretation of this concept corresponds to a relative characterization with respect to some network models, especially Erdős-Rényi (ER), acting as a simple counterpart [2, 3] characterized by homogeneous connectivity.

In particular, these simple reference models are so that the degree of their nodes can be relatively well-predicted from the average of all nodes degrees and controlled just by one parameter: the connection probability, \( p \). Thus, in a sense a simple graph is characterized by degree regularity or homogeneity, having a regular graph as its limit prototype. In this sense, uniformly random networks such as ER can therefore be understood as being statistically regular.

Compared to these regular counterparts, network models such as Barabási-Albert (BA) are understood as being complex, because the degree of the nodes in this type of network is heterogeneous enough so that the properties of the network cannot be properly predicted from the overall average degree (e.g. [1, 4]). As a matter of fact, the degree distribution of the BA model is scale free, implying the existence of nodes, the so-called hubs, with degree substantially larger than the average degree.

It has been shown (e.g. [5, 6]) that degree heterogeneity is not enough to characterize a complex network, in the sense that it is possible to have full regular networks that nevertheless exhibit intricate topology. An example of such network is depicted in Figure 1.

FIG. 1. Example of a network that, though perfectly regular in the sense that each of its \( N = 20 \) nodes have the same degree, \( k = 5 \), cannot be intuitively considered to have a simple overall connectivity structure.
highlight the following two: (i) how to measure the complexity in a broader sense? (ii) what would be the most complex networks that can be obtained?

Our main goal in this work is to investigate these questions. For that, we propose a complexity index that corresponds to the average of the standard deviation of several measurements with a proper correction incorporating the measurements in a comparative manner. Then, we propose an algorithm to maximize the complexity index of a graph having flexible parameters allowing a range possibilities of networks with high complexity.

### II. MATERIALS AND METHODS

Proposing a complexity coefficient based on the diversity of topological measurements creates a necessity to select a group of topological features that can provide a reasonably comprehensive characterization of the network structure (e.g. [1]). However, global proprieties have been avoided because they just give us information about the entire graph instead of its possibly heterogeneous parts. For this purpose, ten topological measurements were estimated for in the network, including: (i) node degree; (ii) average and (iii) standard deviation of the shortest path length for each par of nodes; (iv) clustering coefficient of each node; betweenness centrality for (v) nodes and (vi) edges; (vii) matching index for every pair of nodes that shared an edge; (viii) Laplacian eigenvalues; and (ix) second and (x) third hierarchical degree of each node. Considering the networks to be unweighted and non-directed, we can understand theses measurements as follows:

**Node degree:** the number of the neighbors of a node, quantifying how well a node is connected to other nodes in the graph;

**Shortest path length:** the smallest sequence of adjacent nodes between two nodes in a graph is the shortest path length (or geodesic path length). We consider the average and standard deviation of this measurement taken between each node and all other nodes in the network.

**Clustering coefficient:** information of how well the neighbors of a node are interconnected can be provided by the clustering coefficient [7]. It can be defined as:

\[ C_i = \frac{N_\Delta(i)}{N_3(i)}, \]

where \( N_\Delta(i) \) is the number of all different pairs of nodes that are neighbors of node \( i \) that are connected each other. \( N_3(i) \) is the number of all possible pairs of node \( i \), calculated as \( N_3(i) = k_i(k_i - 1)/2 \). This measurement is taken for each of the network nodes;

**Betweenness centrality:** This measurement provides an indication of how many shortest paths go through the network nodes and edges [8]. It can be expressed as:

\[ B_u = \sum_{ij} \frac{\sigma(i, u, j)}{\sigma(i, j)}, \]

where \( \sigma(i, u, j) \) presents how many shortest paths exist between the distinct nodes \( i \) and \( j \) that the node or edge, \( u \), is included; \( \sigma(i, j) \) is the total value of the geodesic paths between \( i \) and \( j \) and the sum is done over all pairs \( i, j \) where \( i \neq j \). This measurement was taken for each node and each edge in the network;

**Matching index:** This measure indicates the similarity between two linked nodes (e.g. [9][10]) in the sense of the relative number of shared neighbors. It can be expressed as:

\[ \mu_{ij} = \frac{\sum_{k \neq i,j} a_{ik}a_{jk}}{\sum_{k \neq j} a_{ik} + \sum_{k \neq i} a_{jk}}; \]

where \( a_{ij} \) is a element of an adjacency matrix and when \( a_{ij} = 1 \) means that the nodes \( i \) and \( j \) are connected;

**Laplacian eigenvalue:** information about the topology of a network can be obtained from spectral methods based on the analysis of eigenvalues and eigenvectors from adjacency matrix of the graph [11][12]. Specifically, we use the Laplacian matrix, defined as:

\[ L = D - A; \]

where \( D \) is the diagonal matrix of node degrees and \( A \) is the adjacency matrix. Using that, it is obtained the Laplacian eigenvalues of the network. As the graphs considered here is non-directed and unweighted, the values of this measurement are positives and just have real parts [13].

**Hierarchical node degree:** Given a node in a network, it is possible to generalize the concept of its degree by considering not only its first neighborhood, but also other subsequent neighborhoods (e.g. [1][14]). In this work, we take the second and third hierarchical degrees of each node in the networks.

#### A. The Complexity Index

As argued in [6], the complexity of a given network does not limit itself to heterogeneity of node degree, and should also encompass the diversity of other topological measurements. In a sense, the more dispersed are all possible such measurements, the more heterogeneous and, therefore, complex the network can be understood to be.

In order to quantify the overall complexity of a given network, it is important to have some complexity index that takes into account several of the respective topological features of the network. In the present work, we propose one overall complexity index, henceforth referred to as:

\[ B_u = \sum_{ij} \frac{\sigma(i, u, j)}{\sigma(i, j)}, \]

...
to as CI, that is derived from the standard deviations of several measurements, $\sigma_m$. Indeed, each of these standard deviations provides on itself some indication of the complexity of the network regarding that respective feature. Observe that these measurements may be respective to each node or each edge. Therefore, first we obtain several such standard deviations characterizing the heterogeneity of the topological properties of a given network, one respective to each of the adopted topological measurements.

One important point when trying to quantify the complexity of a given network is that this concept is relative to other networks. In other words, one type of network can be said to be more complex than other types, while it remains a difficult problem to express its complexity in an absolute manner. Therefore, in the present work we take into account, while estimating the complexity index of a given network, not only the network whose complexity index is being calculated, but also all the other networks taken as reference.

Because each topological measurement can have a distinct scale of variation (for instance, the average degree is typically larger than 1, the clustering coefficient varies from 0 to 1), it becomes necessary to normalize the values of the considered measurements. Here, we resource to the standardization of each adopted measurement $m$, which can be obtained as follows:

$$z_m = \frac{m - \mu_m}{\sigma_m};$$

where $\mu_m$ and $\sigma_m$ are, respectively, the average and standard deviation of measurement $m$.

Observe that the standardization is performed considering not only the network whose complexity index is being calculated, but also all the other networks taken as reference.

The standard deviations of each measurement obtained for the network of interest after standardization now need to be combined in order to obtain a single complexity index. Ideally, a maximally complex network would have equally large standard deviations for all considered measurements. Consequently, any difference between the standard deviations will reduce the overall network complexity, as understood in the present work.

Let’s represent the largest standard deviation (please refer to Figure 2) by $\sigma_{\text{max}}$, i.e.:

$$\sigma_{\text{max}} = \max_{m=1,M} (\sigma_m).$$

For each measurement $m$, we can define the difference between the maximum standard deviation and the observed respective standard deviation as $\delta_m = \sigma_{\text{max}} - \sigma_m$. Thus, the sum $\Delta$ of differences $\delta_m$ can be expressed as:

$$\Delta = \sum_{m=1}^{M} \delta_m.$$  \hfill (7)

A preliminary index $\alpha$ can now be defined as:

$$\alpha = \frac{\beta - \Delta}{\beta}.$$  \hfill (8)

This index expresses the relative complexity of the network of interest. It will be maximum, $\alpha = 1$, when $\Delta = 0$, indicating that all measurements have the same dispersion. However, any difference $\delta_m$ observed for each measurement $m$ will contribute to increase $\Delta$ value, and therefore, to reduce the value of $\alpha$. In particular, the smallest relative complexity will be obtained when all standard deviations, except one of them, will be zero. In this case, we have $\Delta = \sigma_{\text{max}} = \beta$, implying $\alpha = 0$. Therefore, we have that $0 \leq \alpha \leq 1$.  

FIG. 2. Construct taken into account for defining the complexity index. Each line corresponds to the standard deviation of each of the standardized measurements observed for the network whose complexity is to be quantified. The maximum standard deviation defines a bounding rectangle from which the standard deviation differences $\delta_m$ can be obtained. The maximum relative complexity of 1 is understood to take place when no such differences are observed.
Now, we can proposed an absolute overall complexity index, $CI$, as being equal to the relative complexity index times the average standard deviations observed for the network of interest:

$$CI = \alpha \langle \sigma \rangle.$$  \hfill (9)

In order to better understand the difference between the relative and absolute indices, let’s consider two networks, all of which having all standard deviations identical to 10 and 100, respectively. Though both these networks will have maximum relative complexity $\alpha$, the second network is plainly more complex because of the larger values of its measurement dispersions. This difference is properly reflected in the absolute complexity index, which will result much larger for the second situation.

B. Seeking for complexity

It is interesting to approach our search for highly complex networks as an optimization taking place over a given domain, in the specific case of this work a considerably large space of possible reconstructions of the network edges. As we seek for networks with maximum complexity, the complexity index $CI(G)$ of a network $G$, calculated at each optimization step, is adopted as the function to be maximized. The configuration space is explored through random incremental changes in the network topology. The approach to changing the connections consists of simply choosing an edge $(i,j)$ randomly (with uniform probability), deleting the $j$ node, and then connecting the node $i$ with another node also chosen with uniform probability while not allowing self-loops, connections with nodes that are already neighbors, as well as not leaving $j$ disconnected.

Gradient descent can be used to implement the sought optimization. The complexity of the new graph, $G_{t+1}$, is compared with the current one, $G_t$, as can be seen in Figure 3. If the complexity of the new configuration is larger, it becomes the current graph and the process is repeated. Otherwise, the candidate configuration is ignored and the processing is repeated. Two stop conditions are set. The principal one is the number of new graphs that are accepted. The second is aimed at limiting the total number of iterations in order to avoid that the algorithm runs indefinitely. The resulting networks are called hypercomplex networks – HCs. The algorithm, as well as the types of choices that can be made, are shown in Figure 3.

III. RESULTS

In order to compare the obtained HC networks with other reference theoretical network models, we considered the ER, BA, Waxman (WAX), Random Geometric Graph (RGG) and Watts-Strogatz (WS) structures having the same number $N = 500$ of nodes and same average degree $\langle k \rangle = 8$ (with $\pm 5\%$ of tolerance) as the obtained HC networks. In the case of the WS model, it was taken with respect to 2 different reconnecting probabilities, namely 10% and 100%. For each one of these models, a total of a hundred graphs is taken into account for the sake of statistical significance. Only the network realizations not including disconnected components have been taken into account.

The starting points for the HC derivation method were...
taken as corresponding to ER networks, so that no initial
topological biases be implied by these structures thanks
to the statistical uniformity of the ER model. For refer-
cing purposes, we have taken the HC networks after
1000, 2000, 3000 and 4000 taken optimization steps, and
these networks are henceforth referred to as HC-1000,
HC-2000, HC-3000, and HC-4000, respectively.

Principal component analysis (PCA [15, 16]) has been
applied on all 10 topological measurements of the con-
sidered networks so as to project the networks into two
dimensions, allowing respective comparative visualiza-
tion. The results are shown in Figure 4. The ob-
tained 96.1565% variance explanation corroborates the
relevance of the PCA projection. The CI respective to
each network is also shown in terms of the heatmap.

Several interesting results can be inferred from Fig-
ure 4. First, we have that each of the considered network
model yielded a respective cluster that, despite its intrin-
sic dispersion, is well-separated from the others. Then,
and more important, as a consequence of the subsequent
optimization steps, the group respective to the HC net-
works defined an unfolding, starting at the ER models,
that is characterized by increasing values of CI, toward
a previously empty (low density) region in the PCA. In-
terestingly, the ‘trajectory’ respectively defined tends to
move away from all other models, including BA, therefore
suggesting that the topology of the HC is distinct
from those models.

The obtained results corroborate not only that the HC
model is more complex than the other considered types of
networks (according to the adopted CI), but also that the
HC structures displace themselves towards a configur-
ation that is substantially different from the other models.
In order to better understand the subsequent changes in
the properties associated to the HC model, we present in
Figure 5 the average ± standard deviation of each con-
sidered topological measurement along the optimization
steps applied to obtain the HC networks.

Interestingly, the optimization dynamics tends to in-
crease the standard deviation respectively to most of the
adopted measurements, corroborating its effectiveness in
deriving networks that are more complex respectively to
the overall set of topological features, not only the degree,
as can be seen in Figure 5. The CI observed for 4000 re-
alizations of the optimizations is shown in Figure 6, also
increasing with the optimization steps.

Figure 7 presents the visualizations of the HC evolution
with $N = 500$ nodes and $\langle k \rangle = 8$, from ER to opti-
max stage 8000. Some interesting features can be iden-
tified in this figure, including low clustering coefficient,
at least at its periphery, as well as a gradient of degree
extending from the network center toward its periphery.
Also interesting is the tree-like structure appearing at the
border of the network. These obtained structural com-
plexities were absent from the original ER structures.
The obtained HCs present some additional surprising topological properties such as larger diversity of degree and peripheral branches, properties nonexistent in the comparative network models. However, the degree distribution obtained for the HCs is only slightly broader than that of the ER counterparts, we can conclude that the enhanced complexity of the HC network stems not only from the degree distribution, but also from the heterogeneity of all other considered topological measurements, which have indeed been quantitatively observed to have their respective CVs increasing with the interactions.

In the present work, we aimed at further enhancing the complexity of networks. In order to do so, we started from the fact that the complexity of a network derives not only from heterogeneous degree distributions, but also of present heterogeneity of other, preferably most, other topological measurements [5, 6]. First, we defined an overall index reflecting the heterogeneity of a large number of topological measurements taken on the given network. More specifically, this complexity index $CI$ expresses the relative dispersion of each considered measurement with respect to their maximum value, so that it reaches its maximum value when all measurements have maximum dispersion. Then, we apply an optimization procedure, starting with a uniformly random network (ER), and performing gradient descent over the negative CI of the respectively obtained network. More specifically, this complexity index $CI$ expresses the relative dispersion of each considered measurement with respect to their maximum value, so that it reaches its maximum value when all measurements have maximum dispersion. Then, we apply an optimization procedure, starting with a uniformly random network (ER), and performing gradient descent over the negative CI of the respectively obtained network. More specifically, this complexity index $CI$ expresses the relative dispersion of each considered measurement with respect to their maximum value, so that it reaches its maximum value when all measurements have maximum dispersion. Then, we apply an optimization procedure, starting with a uniformly random network (ER), and performing gradient descent over the negative CI of the respectively obtained network. More specifically, this complexity index $CI$ expresses the relative dispersion of each considered measurement with respect to their maximum value, so that it reaches its maximum value when all measurements have maximum dispersion.

Several interesting results have been obtained. More specifically, we have that, as the number of optimization modifications are taken, the HC networks tend to perform a well-defined trajectory in the PCA obtained from several respective topological measurements. This trajectory, which is indeed more similar to elongated clusters, has been observed to head toward a low density position in the PCA space, departing from all the other considered theoretical network models. As expected, the $CIs$ of these networks tend to increase progressively.

The obtained HCs present some additional surprising topological properties such as larger diversity of degree and peripheral branches, properties nonexistent in the comparative network models. However, the degree distribution obtained for the HCs is only slightly wider than node regularity.

To a good extent, the area of network science derives its motivation from complexity studies, such as the identification of the BA model as a network presenting node degree heterogeneity, more specifically nodes degree distributions following a power law. Indeed, the very concept of complex network stems from comparisons with relatively ‘simple’, homogeneous counterparts such as the ER model whose nodes tend to have degree values similar to the average node degree, indicating a kind of statistical

FIG. 5. Average ± standard deviation of the several considered topological measurements of HC networks with $N = 500$ nodes and $\langle k \rangle = 8$ along the taken optimization steps (interaction). Observe also that the dispersion of the node degree (as well as the Laplacian eigenvalues and second hierarchical degree) tended to saturate and even decrease, indicating that the complexity of the obtained network could not be obtained by considering only this measurement.

FIG. 6. Average ± standard deviation of the $CI$ observed during the optimization procedure adopted for generating HC networks with $N = 500$ nodes and $\langle k \rangle = 8$ in terms of the taken optimization steps (interaction). Given that the degree distribution obtained for the HC networks is only slightly broader than that of the ER counterparts, we can conclude that the enhanced complexity of the HC network stems not only from the degree distribution, but also from the heterogeneity of all other considered topological measurements, which have indeed been quantitatively observed to have their respective CVs increasing with the interactions.
that obtained for ER counterparts. Thus, in a sense the HC networks are not much more complex than ER networks from the perspective of degree distribution. However, at the same time HCs tend to present topology different from all other models, and are characterized by the largest obtained CIs. This indicates that the complexity of HCs, as had been initially postulated, derives from the heterogeneity not only of node degree, but also of the other considered topological measurements.

The reported work paves the way to a number of related developments, many of which are currently being pursued. First, it would be interesting to start from theoretical complex network models other than ER. It could be expected that these other models, by being less homogeneous, could imply an initial bias that may or may not correspond to that to be taken by the HCs. In the former case, the changes toward maximum complexity would therefore be delayed so that the initial bias could be first overcome. Another interesting research line concerns the study of the surprising appearance of peripheral branching subnetworks, provided a substantially large number of steps is allowed. These new structures probably imply in an abrupt change of the trajectory underwent by the HCs in the PCA space. It remains a subject of great interest to further study this second modification stage presented by the HCs.

Another interesting aspect would be to further study the convergence of specific topological features, such as the degree and its hierarchies, as they may indicate critical steps along the optimization dynamics. Given that directionality and weights are known to strongly influence not only the network structure, but also respective dynamics undergoing in these networks, it would be interesting to extend the present work to incorporate those types of networks.

It would also be interesting to consider alternative complexity indices. Indeed, though the adopted CI reflects the overall heterogeneity of the network topological features. Yet another promising possibility is to compare the HC networks with real-world structures, in order not only to try to identify analogue situations, but also to better understand, in a comparative manner, their relative overall complexity.

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FIG. 7. An HC network with for $N = 500$ nodes and average degree $\langle k \rangle = 8$ that was allowed to undergo optimization up to 8000 steps. The diameter of the nodes has been represented as being proportional to the respective degree. New peripheral structure, mostly branching subnetworks, are progressively incorporated.