Modeling the Perspectives for Scientific Advancement

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Abstract

The development of science constitutes itself an important subject of scientific investigation. Indeed, better knowledge about this intricate dynamical system can provide subsidies for enhancing the manners in which science progresses. Recently, a network science-based approach was reported aimed at characterizing and studying the prospects for scientific advancement assuming that new pieces of knowledge are incorporated in a uniformly random manner. A surprising result was reported in the sense that quite similar advancements were observe for both Erdős–Rényi (ER) and Barabási–Albert (BA) knowledge networks. In the present work, we develop a systematic complementation of that preliminary investigation, considering an additional network model, the random geometric graph (GR) as well as several other manners to incorporating knowledge, namely preferential to node degree, preferential to closer or adjacent nodes, as well as taking into account the betweenness centrality of the unknown nodes. Several interesting results were obtained and discussed, including: the uniform strategy led to the best expansion in the GR model, the results of the degree and betweenness expansion for the ER and GR models were similar to those obtained using uniformity method in those same models. Surprisingly, the BA model led to just a slightly faster expansion than in the uniform case. Though qualitatively similar, strategies based on the degree and betweenness yielded distinct results as a consequence of them not being linearly related.

1 Introduction

Science can be approached and studied as a complex system whose dynamics take place over space and time. Along centuries, or even millennia, science has progressed from relatively simple concepts – typically covered as a single discipline – to a universe of specialized areas involving highly sophisticated models and theories.

At any given time, great attention is often given to identifying the prospects for scientific advancement, which are understood in a somewhat subjective manner as corresponding to the number and importance of the potential developments that can be achieved in the light of the existing knowledge. The accurate identification of these prospects is of particular interest because they help focusing and prioritizing research and funding resources along specific venues that
are more related or of particular relevance in a given time and location.

The impressive development of the area known as network science (e.g. [12]) (roughly speaking, the study of complex networks) was to a great extent a consequence of the generality of graphs (also known networks) for representing virtually every discrete system (e.g. [4]), ranging from the Internet to molecules interaction. Indeed, it is even possible to represent the scientific body of knowledge as a complex network, e.g. by representing portions of knowledge as nodes while expressing the respective relationships in terms of edges (e.g. [5, 14]).

Such representations of scientific knowledge in terms of networks have paved the way to a number of interesting possibilities in scientometrics, the science that studies science (e.g. [10, 13, 15, 2]). For instance, it becomes possible to model scientific advancement in terms of different types of random walks along these representations (e.g. [11, 3]). It also becomes possible to model and simulate the transmission of information and knowledge (e.g. [9, 8]).

Complex network representations of scientific knowledge also provide subsidies for the main motivation of the present work, namely the definition and quantification of the prospects for scientific advancement. In a preliminary work [6], having represented the overall scientific knowledge as a complex network, a subset of these nodes was understood as the nucleus, representing the currently known portion of the knowledge. Then, the prospects, or potential for knowledge advancement at that particular stage could be objectively defined and quantified as deriving from the number of yet unknown nodes that can be accessed from the nucleus. More specifically, the indices $r$ and $s$ were defined. Index $r$ indicates the prospect of knowledge expansion around the nucleus, while index $s$ is associated with a redundancy of the knowledge advancement.

As described in [6], it is not only possible to quantify the potential for scientific advancement with respect to the current stage, but also to study how this potential unfolds as the nucleus is progressively expanded, e.g. by selecting new node with uniform random probability. In those circumstances, a remarkable result was observed, namely that the prospects do not depend on the topology of the network (two models with quite different topological properties, namely Erdős–Rényi (ER) and Barabási–Albert (BA), were considered in [6]).

One of the objectives in [6] was to study the change of $r$ with the size $c$ of the nucleus. It was shown that a typical curve has two parts: it increases with the increase of $c$, achieves a maximum $r_{\text{max}}$ at $c_{\text{rmax}}$ and then steadily decreases with $c$ until $r = 0$. When a curve has a lower $c_{\text{rmax}}$ compared to another, it means that it achieves the maximum value of $r$ for a smaller value of $c$. That is to say that it achieves the optimal value of the potential knowledge expansion with a smaller nucleus size.

The surprising result that quite similar prospects were observed for varying topologies was understood to be a consequence of the uniformly random choice of nodes to be incorporated into the nucleus, and it was foreseen that other strategies of nucleus expansion could lead to distinct results.

The present work resumes and expands those investigations. Not only we consider additional complex networks models, namely the random geometric graph (GR) but more importantly we study other manners of expanding the nucleus preferentially in terms of degree, distance, adjacency and betweenness centrality.
Interesting results are obtained, including the surprising effectiveness of the uniform expansion strategy on the GR model, the fact that the degree strategy was just slightly more efficient in the BA model than the uniform strategy, as well as the large variation in the results observed on the GR model depending on the chosen strategy.

This work starts by presenting the adopted data and basic methods, including models and properties of complex networks. Then, the main framework employed for modeling the unfolding of the prospects of scientific advancement is described, including the measurements that are used for respective quantification. The main obtained results are then respectively presented and discussed.

2 Data and Methods

The ER model is among the most frequently studied network type. One of the proposed procedures to obtain these networks consists in starting with an isolated set of vertices and then gradually adding edges with uniform probability among all the possible edges. In this construction scheme, given a fixed number of vertices, and a desired number of edges, all graphs are equally probable.

The GR model is another category of random graphs in which the specification of the position of the vertices in a given metric space is performed in random manner. The edges are then deterministically created by linking vertices at most a given distance apart. This procedure leads to the generation of clusters of vertices with high modularity, which do not appear in the ER model.

Despite the interest motivated by the simplicity of these networks, there are relatively few real-world structures that can be respectively modeled. In particular, it has been noted that real networks have uneven degree distribution. In this context, the BA model was proposed as being capable of generating power law degree distributions. Such networks are also called scale-free (or scale invariant) networks. The construction of a BA model consists in a growth model following a preferential attachment rule, which is linear to the degree of the candidate vertices. This rich gets richer phenomenon principle leads to the generation of a few highly connected nodes — the hubs.

The complexity characterizing many network models motivated the development of a myriad of measurements. One of most basic measurements is the vertex degree, which in an undirected network represents the number of connections of the vertex. Network topologies can be initially compared based on their degree probability distribution over the network. In different applications, such as epidemics and urbanism, it is often useful to identify the most important vertices. The concept of importance is application-dependent, giving rise to multiple approaches to centrality characterization. The betweenness centrality is one of these measurements, based on the shortest path measurement. More specifically, it counts the number of shortest paths that pass through each vertex.

3 The Proposed Framework

Being composed of a set of concepts and inter-relationships, knowledge can be effectively represented in terms of a network or a graph. Having decided how the portions of knowledge are to be assigned to nodes, which involves choosing a respective level of detail, one maps each of these
portions as a node, while interrelationships are
represented in terms of respective edges. There
are several types of interrelationships that can
be considered, including pre-requisites (e.g. one
need first to learn topic A before proceeding to
topic B), application of theorems and results, or
simply a citation of words associated to the cho-
sen topics.

Once knowledge is organized in this man-
ner, we can represent its portion that is already
known in terms of the respective nodes, which
gives rise to the concept of nucleus. Though
other approaches can be adopted, in this work
we consider all the interconnections between the
known nodes. Therefore, all nodes other than
those belonging to the nucleus correspond to
pieces of the knowledge that are not yet known,
being associated to the perspectives for scientific
advancement. The progress of our understanding
of the knowledge represented in the overall net-
work can therefore be understood as the progres-
sive incorporation of previously unknown nodes
into the nucleus, which is consequently expanded
until all nodes are encompassed.

We propose to study the dynamics of the
prospect for scientific advancement as we in-
crease the nucleus by using two different mea-
surements, \( r \) and \( s \), as previously proposed in [6].
The measurement \( r \), defined as the ratio between
the number of nodes adjacent to the nucleus not
yet visited \( (n) \) and the total number of nodes
\( (N) \), i.e.:

\[
 r = \frac{n}{N}, \quad (1)
\]

This measurement can be seen as a relative
indication of the prospect for scientific advan-
cement. The other proposed measurement, \( s \), de-
defined as the ratio between the number of \( n \) and
the number of edges that connect the nucleus to
these adjacent nodes not yet visited, i.e.:

\[
 s = \frac{n}{e} \quad (2)
\]

In Figure 1, the nucleus is represented by the
set of the \( n \) red nodes. The yellow nodes repre-
sent the adjacent nodes and the green ones rep-
represent the non-discovered nodes. The edges be-
tween the nucleus and the adjacent nodes is de-
noted by \( e \). In the example shown, the nucleus is
composed of three vertices and \( r = n/N = 4/17 \)
and \( s = n/e = 4/5 \).

However, not all these unknown nodes are
likely to be equally accessible from nodes in the
nucleus, which gives rise to several distinct pos-
sibilities of expanding the nucleus. Figure 2 il-
lustrates this effect in terms of the measurement
\( s \).

The most elementary possibility, already con-
considered in [6] consists of choosing unknown nodes

Figure 1: Calculation of the proposed measure-
ments in an example network. The green nodes
represent knowledge not yet discovered, the red
ones represent the nucleus, and the yellow nodes
represent the knowledge adjacent to the nucleus.
In this example, \( N=17, n=4 \) and \( e=6 \) and hence,
\( r = 4/17 \) and \( s = 4/5 \).
in uniformly random manner for respective incorporation into the nucleus. Another interesting possibility is to choose among the unknown nodes with probability proportional to their respective degree, reflecting a tendency that pieces of knowledge with more interconnections are more likely to be discovered.

It is also interesting to consider expansion strategies relying on the distance or adjacency between nodes. For instance, nodes that are closer to those belonging to the nucleus can be assumed to be more likely to be learned, according to a respective probabilistic model. Alternatively, unknown nodes that are adjacent to the nucleus (i.e. directly connected to at least one of the nucleus nodes) can be chosen as the next pieces of knowledge to be discovered.

It is also interesting to consider the betweenness centrality of the network vertices. In this manner, it is possible to derive a nucleus expansion strategy that takes into account the number of shortest paths going through each node, taking into account the possible interrelationships between the pieces of knowledge in the overall network.

In this work, we adopted all the above motivated methodologies for progressively extending the nucleus. More specifically, we have: (i) unknown nodes are chosen with uniform probability; (ii) preferential to the vertex degree; (iii) with probability \( p(v) = \alpha \cdot \exp(-\beta d) \), where \( d \) is the distance; (iv) the unknown nodes connected (adjacent) to the nucleus are chosen with uniform random probability; and (v) preferential to the betweenness centrality.

Figure 3 illustrates the signatures of the measurements \( r \) and \( s \) typically obtained in our simulations. As every signature of \( r \) is qualitatively similar, it is enough to characterize these curves in terms of the two measurements \( r_{\text{max}} \) and \( r_{\text{max}} \) indicated in Figure 3 corresponding to the position where the peak of \( r \) is observed and the value of this peak.

In the case of the signatures obtained for \( s \), which are also all qualitatively similar, we express the intensity of the decrease of \( s \) in terms of the value of \( c \) where the value of \( s \) falls from 1 to \( 1/\sqrt{2} \approx 0.707 \), as frequently adopted in physics and engineering.
4 Results and Discussion

We performed three main experiments, in which we varied the size and average degree of the network according to the following configurations: (1) $N = 300$ and $\langle k \rangle = 12$; (2) $N = 300$ and $\langle k \rangle = 18$; and (3) $N = 700$ and $\langle k \rangle = 12$.

Figure 4 depicts the scatterplot of $r_{\text{max}}$ versus $c_{r_{\text{max}}}$. This results indicates that these two measurements are strongly interrelated, so that our analysis will concentrate on the former measurement (i.e. $r_{\text{max}}$). The dispersion in Figure 4 can be observed to be stronger when $r_{\text{max}}$ is small and $c_{r_{\text{max}}}$ is large. In other words, the position where smaller peaks are observed is more difficult to be predicted from $c_{r_{\text{max}}}$.

Therefore, the following discussion focuses on the measurements $r_{\text{max}}$ and $c_{s0}$.

Each of these experiments are respective to the ER, BA, and GR theoretical models of complex networks, and five strategies for controlling the expansion of the kernel, namely uniformly random, dilation, preferential to the degree, to the betweenness centrality, and to the distance.

The results obtained are depicted in Figure 5.

The results were found to be similar for different network sizes and average degrees, with the exception of the expansion strategy based on the distance, in which case the $r_{\text{max}}$ increases with the network size for the considered network sizes. All other results are qualitatively similar with the network size, and are therefore discussed together in the following.

As could be expected, the results for the uniform expansion strategy were similar to those obtained in [6]. It is interesting to note that the uniform method led to the best expansion in the GR model. This model had not been considered in [6]. Regarding the degree expansion strategy, the results for the ER and GR models were similar to those obtained in the uniform case. Surprisingly, the BA model resulted in just a slightly faster expansion than in the uniform case. The results for the distance-based expansion strategy were similar to those obtained for the BA and ER models using the uniform strategy. Contrariwise, the expansion was much slower for the GR model when the distance approach was employed. This contrast between the models is likely due to the difference in diameter between the networks generated by the models. In the case of the ER and BA networks, almost all nodes can be reached from the nuclei after two steps for the considered network sizes. In the GR model a distinct behavior is observed, the knowledge becomes localized around the nuclei, and expands by an amount that is associated with the size of the nuclei periphery.

Regarding the dilation strategy, the results were similar to those obtained by the distance-
based expansion, but were more pronounced in the sense that it represented the worst expansion strategy among all models. The results for the betweenness strategy were similar to those obtained by the uniform strategy in the ER and GR models. Interestingly, the betweenness led to the best expansion strategy in the BA model, being even better than the degree approach. This happens because the betweenness grows very fast as the degree of the nodes increase. Actually, it has a superlinear relationship with the degree, as can be seen in Figure 6. This means that hubs will have a disproportionately large preference during the knowledge expansion, leading to a better coverage of the network.

It is important to note that all expansion strategies led to similar results in the ER model. This is because the vast majority of the nodes have similar properties for this model. On the other hand, the results for the GR model were highly dependent on the strategy used. Even though the BA model is known for being heterogeneous [1], the GR model had a higher impact on the considered strategies depending on the node property used. This is likely due to the large diameter of the networks generated by the model, which allows highly distinct expansion dynamics according to the knowledge acquisition strategy. The BA model, having small-world properties, does not yield the same variability.

Concerning the measurement $c_{sd}$ shown in Figures 5(d)-(f), though the results vary with the network degree, they have similar relative variations according to the network model. As far as the absolute variations are concerned, the values in (e) are smaller than in (d) because of the increase of average degree, which implies more links to converge on the nodes adjacent to the nucleus. No variation is however observed with the increase of network size from (d) to (f).

Concerning the relative variations, the strategies were found to have similar effects in the case of the ER models, while larger differences were observed for BA, and even larger changes for GR. These effects are analogous to those observed and discussed for the $r_{max}$ measurement. The values for $c_{sd}$ are positively correlated with $r_{max}$ for the BA model, while a negative correlation is observed for the GR model. The values obtained for the ER model are larger than those obtained for the BA and GR. Since the GR model has a large clustering coefficient [7], it is expected that the connections will tend to be more convergent. In the case of the BA model, many nodes in the nucleus will tend to be connected to a hub, lowering the value of $S$.

The effect of the strategies is analogous to that observed and discussed in the case of $r_{max}$, with the difference that the strategies based on dilation and distance were now found to be very similar.

5 Concluding Remarks

From its beginnings, science has relied on the identification of prospects for subsequent advancements, which can not only contribute to better planning but also for making the scientific activity more efficient. Yet, despite such central importance, the issue of defining and identifying the prospects for scientific advancement have been approaches in a predominantly subjective manner.

Representing the continuation of a recently reported preliminary approach to this problem [6], the current work described a substantially extended investigation on how the prospects for scientific advancement can be quantified in a more
objective manner and how it can be predicted given network-based representations of bodies of knowledge.

More specifically, the knowledge is represented as a network by assigning its components to nodes, while the relationships between these components are represented by respective links. Three distinct models have been considered for this finality, namely ER, BA, and GR, each being characterized by specific topological properties. The current knowledge is understood to correspond to a subgraph of the overall network, which is called nuclei. The prospect for advancement of knowledge can then be defined as corresponding to the number of nodes that are adjacent to the nuclei.

By adopting several different strategies for expanding the nuclei along time, it became possible to study how the prospects respectively changed. Several interesting results were obtained and discussed. A surprising result was that the uniform strategy led to a relatively good expansion of the nucleus for all models, when compared to the other strategies. Surprisingly, this strategy was the most effective for the GR model. Another interesting result was that despite the heterogeneity of the BA model, similar results were obtained for all expansion strategies. On the other hand, the results for the GR model varied broadly according to the strategy used.

The results presented in this work are a first step towards modeling knowledge expansion using complex networks. Furthermore, the proposed dynamics is not limited for modeling knowledge expansion and can be applied to other areas. For instance, an interesting prospect is to quantify the accessibility of cities using the proposed $r$ and $s$ indices on road networks.

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Figure 5: Comparison among the topologies and the different strategies of increase of the nucleus based on the two proposed measurements. In the first row and in the second rows consider the measurement r and s, respectively. The columns represent different graph parameters: (300, 12), (300, 18), (700, 12), for the first, second and third columns respectively, with \((n, k)\) representing graphs with \(n\) vertices and average degree \(k\).
Figure 6: Correlation between the vertex degree and the betweenness centrality for all the experiments with topology BA.