Reverse engineering of linking preferences from network restructuring

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We provide a method to deduce the preferences governing the restructuring dynamics of a network from the observed rewiring of the edges. Our approach is applicable for systems in which the preferences can be formulated in terms of a single-vertex energy function with \( f(k) \) being the contribution of a node of degree \( k \) to the total energy, and the dynamics obeys the detailed balance. The method is first tested by Monte Carlo simulations of restructuring graphs with known energies; then it is used to study variations of real network systems ranging from the coauthorship network of scientific publications to the asset graphs of the New York Stock Exchange. The empirical energies obtained from the restructuring can be described by a universal function \( f(k) \sim -k \ln k \), which is consistent with and justifies the validity of the preferential attachment rule proposed for growing networks.

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I. INTRODUCTION

In the past few years, the analysis of the network structure of complex systems has become a rapidly expanding interdisciplinary field [1–3]. Interpreting the dynamics of these complex networks with techniques developed in statistical mechanics represents a new approach to network theory [4–11]. A recently introduced method is to define equilibrium network ensembles as stationary ensembles of graphs generated by restructuring processes obeying detailed balance and ergodicity [11]. During such a restructuring process, edges are removed and/or inserted. If an energy function of the graphs is also given, then the construction of the corresponding microcanonical, canonical, and grand canonical ensembles can be carried out in a similar way as in classical statistical physics. However, unlike in many physical systems, the energy of a graph cannot be derived from first principles and does not necessarily exist. In the case of graph ensembles designed to have some prescribed property, a properly defined cost function (or energy) can capture the deviations from this property. This method of defining energy is typically used in optimization contexts.

For network systems, in which the restructuring is assumed to be governed by interactions that can be interpreted in terms of energy, one can try to deduce this energy using the data obtained from the time series of the evolution of the system. In the present work, our goal is to demonstrate this reverse engineering process in detail. In particular, we shall put our methods into practice for a few different network systems such as the coauthorship networks of scientific publications [12–17], the network of U.S. film actors [18,19], and the asset graphs of the New York Stock Exchange [20].

II. RESTRUCTURING PROCESSES AND PREFERENCES

In the following we assume that the preference for establishing a given link can be expressed in terms of a change in the network’s total energy. During this graph restructuring process, the edges (which can be deleted, relocated, or newly inserted) can be thought of as particles in a physical system and the vertices as the volume of the system. Since the properties of growing networks have already been studied in great detail, here we assume that the number of vertices, \( N \), is fixed.

In the statistical mechanics picture, the time evolution of the probability of occurrence of the graphs is governed by a set of master equations [11]:

\[
\frac{\partial P_a}{\partial t} = \sum_b \left( P_b r_{b\rightarrow a} - P_a r_{a\rightarrow b} \right),
\]

where \( P_a \) is the probability of graph \( a \) and \( r_{a\rightarrow b} \) denotes the transition rate from graph \( a \) to graph \( b \). If the dynamics is governed by an energy function, then it determines the ratio of the transition rates as

\[
\frac{r_{a\rightarrow b}}{r_{b\rightarrow a}} = e^{-(\Delta E_{ab} - \mu \Delta M_{ab})/T}.
\]

In the equation above \( \Delta E_{ab} = E_b - E_a \) is the energy difference between the graphs, \( \Delta M_{ab} = M_b - M_a \) denotes the difference in the total number of edges, \( \mu \) is the chemical potential associated with the appearance of extra edges in the system, and \( T \) denotes the temperature, corresponding to the level of noise. If \( M \) is kept constant, then in the \( T \rightarrow \infty \) limit the dynamics converges to a totally random rewiring process, and thus the ensemble of classical random graphs is recovered [21]. On the other hand, at low temperatures the graphs with lowest energy (meeting the requirements set up by the preferences) are selected with enhanced probability.

As the transition rates obey detailed balance if the dynamics is ergodic, the probability distribution will converge to a stationary distribution.
III. SINGLE-VERTEX ENERGIES

The energy function of a network corresponds to the preferences in the rearranging of the graph structure (e.g., when relocating an edge from one vertex to another). If only the local properties of the graph influence the edge relocation, then the simplest form of the energy is given by the sum of contributions from the individual vertices. Assuming that these contributions depend only on the degrees of the vertices, the total energy can be written as

\[ E = \sum_{i=1}^{N} f(k_i), \]

where \( N \) is the total number of vertices, and \( k_i \) denotes the degree of vertex \( i \). Note that if \( f(k) \) is shifted by a constant, the resulting dynamics remains unchanged since only the difference between energies associated with different degrees may influence the restructuring. Therefore, without loss of generality we may set \( f(0)=0 \). Furthermore, the linear part of \( f \) is irrelevant if the number of edges is constant (since its contribution is proportional to the number of edges in the graph), and simply renormalizes the chemical potential if the number of edges is allowed to change.

An alternative form of the single-vertex energy functions can be written as

\[ E = \sum_{i=1}^{N} \sum_{i'} g(k_{i'}), \]

where \( i' \) runs over all vertices that are neighbors of vertex \( i \). In this interpretation, the energy of an individual vertex depends on the connectivities of its neighbors, and vertex \( i \) collects an energy \( g(k_{i'}) \) from each of its neighbors. These neighbors in turn will all collect \( g(k_i) \) from vertex \( i \); therefore, the total contribution to the energy from vertex \( i \) is \( k_i g(k_i) \). Thus, by choosing

\[ f(k) = k g(k), \]

the two alternative forms of the single-vertex energy, Eqs. (3) and (4), become equivalent.

The advantage of the latter representation is that the irrelevant linear part of \( f(k) \) appears as a simple additional constant term in \( g(k) \) for \( k \gg 1 \).

IV. REVERSE ENGINEERING WITH INDEPENDENT EDGE DYNAMICS: THE METHOD

In the following we assume that the energy function of the investigated system falls into the class of the single-vertex energy functions (4). The main point of our method is that it assumes independent dynamics for each half edge. In this approach, each vertex \( i \) is treated as a hedgehog, with \( k_i \) half edges. Since the energy function depends only on the degree sequence, the energy of the network is identical to that of the set of isolated hedgehogs. The restructuring of the network can be approximated by the insertion and deletion of half edges. This approximation is valid when the number of vertices is large compared to the typical number of half edges on the individual vertices. Let us denote by \( r_{k \rightarrow k-1} \), the rate at which existing half edges on vertices with degree \( k \) disappear, and accordingly by \( r_{k-1 \rightarrow k} \) the rate at which new half edges appear on vertices with degree \( k-1 \). The ratio of these two rates is determined by the energy in a way similar to Eq. (2):

\[ \frac{r_{k \rightarrow k-1}}{r_{k-1 \rightarrow k}} = \frac{e^{f(k)-\mu k}}{e^{f(k-1)-\mu(k-1)}} T, \]

where \( \mu = \mu/2 \) denotes the chemical potential for the half edges. From Eq. (6) it is clear that the effect of the chemical potential on the dynamics cannot be separated from the effect of the linear part of \( f(k) \), and the multiplication of \( f(k) \) and \( \mu \) by the same number is equivalent to the rescaling of the temperature. For these reasons it is convenient to introduce the dimensionless single-vertex energy

\[ \phi(k) = \frac{f(k) - \mu k}{T}, \]

which incorporates the chemical potential as well. This yields

\[ \frac{r_{k \rightarrow k-1}}{r_{k-1 \rightarrow k}} = e^{\phi(k)-\phi(k-1)}, \]

The number of disappearing edges on vertices with degree \( k \) per unit time can be written as

\[ I_{k \rightarrow k-1} = r_{k \rightarrow k-1} p_k N_k, \]

because there are \( p_k N \) vertices with \( k \) edges and these have a total of \( p_k N_k \) edges on them. Similarly, the current between the same two states in the opposite direction is

\[ I_{k-1 \rightarrow k} = r_{k-1 \rightarrow k} p_{k-1} N_{k-1}, \]

because there are \( p_{k-1} N \) vertices with \( k-1 \) edges and the appearing new half edge can be placed at \( N-1 \) different positions (corresponding to the \( N-1 \) possible neighbors of a given vertex). For simple graphs (i.e., when only zero or one connection is allowed between two vertices) the number of these possible positions is \( N-1-(k-1) \) and accordingly the \( (N-1) \) factor in expression (10) should be replaced by \( (N-k) \). However, in all cases studied in this paper we have \( N \gg k \), and therefore we may use

\[ I_{k \rightarrow k-1} = r_{k \rightarrow k-1} p_k N_k, \]

in all situations. From the ratio of the currents (11) and (9) and Eq. (8) we get

\[ e^{\phi(k)-\phi(k-1)} = \frac{I_{k \rightarrow k-1} p_k N_k}{I_{k-1 \rightarrow k} p_{k-1} N_{k-1}}. \]
FIG. 1. We illustrate the measurement of the currents $I_{k \rightarrow k+1}$ and $I_{k \rightarrow k-1}$ in the data set by comparing two subsequent states of vertex 0 in a hypothetical simple graph with 17 vertices. (Only edges connected to vertex 0 are shown.) In the initial state (left side), the central vertex is connected to vertices 1,2,4,5 with one edge and to vertex 3 with two edges; hence its degree is $k=6$. In the second state (right side), the link to vertex 2 and one of the links to vertex 3 disappeared giving a contribution $I_{k-5}=2$ to the currents. Similarly, new links to vertices 6, 12, and 13 appeared; thus $I_{k+7}=3$.

In the alternative representation of the energy defined in Eqs. (5) and (6), one can introduce

$$\gamma(k) = \frac{\phi(k)}{k} = \frac{g(k) - \bar{\mu}}{T}. \quad (14)$$

V. CASE STUDIES

We first tested our method on known energy functions used in Monte Carlo simulations, and then applied it to study real world systems ranging from the coauthorship networks of scientific publications to the asset graphs of the New York Stock Exchange. In each case, the statistics of vertices with a given degree became poor with increasing $k$; therefore only the interval of the well represented degrees was taken into account in our reverse engineering process. The upper boundary of this interval, $k_{\text{max}}$, was set to the point where the time average of the number of vertices with degree $k$ became smaller than 0.1% of the average number of vertices.

As explained in the previous sections, when the total number of edges, $M$, is fixed, the linear part of $f(k)$ is irrelevant. When $M$ is allowed to vary, a linear function $-\bar{\mu}k$ naturally appears in Eq. (2), and cannot be uniquely separated from the energy. Therefore, we will focus on the nonlinear part of the empirically obtained $\phi(k)$, corresponding to the nonlinear part of the single-vertex energy. In general, the $\phi(k)$ obtained from the data can be decomposed into

$$\phi(k) = C_0 + C_1 k + \phi^*(k), \quad (15)$$

where $\phi^*(k)$ denotes the nonlinear part of $\phi(k)$. The additional $C_0$ constant shift is introduced to account for the irregular behavior of the energy of vertices with zero degrees in the collaboration networks (the networks of scientific publications and U.S. movie actors). In these systems $\phi(k)$ is relatively smooth for $k \geq 1$ in contrast to a gap in the energy observed between $k=0$ and $k=1$. Accordingly, $k=0$ has been excluded when fitting the empirical results, and the shift of the $k=1$ part caused by the gap is taken into account with the help of $C_0$. The $\gamma(k)$ corresponding to Eq. (15) can be written as

$$\gamma(k) = C_0/k + C_1 + \gamma^*(k). \quad (16)$$

where $\gamma^*(k)=\phi^*(k)/k$. In the expression above, the first term decays for high $k$ and the second is a constant; therefore, in practical cases the remaining nonlinear part is somewhat more apparent than in the $\phi(k)$ representation.

In the figures showing our results, we shall plot $\phi(k) - C_1 k$ and $\gamma(k) - C_0/k - C_1$, since in this way both the nonlinear part of the energy and the gap at $k=0$ for the collaboration networks become apparent.

A. Testing with known energy functions

We first tested our method on known energy functions used in Monte Carlo (MC) simulations with a constant ($N = 10000$) number of vertices and $\langle k \rangle = 2$. The most trivial choice for the energy function was the case when no energy was present in the rewiring and the edges were replaced randomly. In this case the network converges to a classical random graph regardless of the initial state, and accordingly the maximum degree taken into account in the reverse engineering process was $k_{\text{max}}=7$. The other tested energy was chosen to be $f(k) = -k \ln(k)$. This choice was motivated by our previous studies which showed that in this system, around $T = 1$ a scale-free degree distribution can be observed [10]; hence the interval of $k$ taken into account in the reverse engineering is wider ($k_{\text{max}}=27$) than in the case of random rewiring.

Figure 2 shows our results for the two test energies. In both cases, $C_0$ was set to zero, and $C_1$ was set equal to $\phi(1)$ [since both energies used in the MC simulations give $f(1) = 0$]. In both situations, the resulting empirical $\phi^*(k)$ could be fitted well with the energy used in the MC simulation.

B. Collaboration networks

The collaboration networks investigated in this paper can be listed as follows: the coauthorship networks of neuroscience and math publications, the coauthorship networks of the Los Alamos e-print archives of Condensed Matter, High Energy Physics—Phenomenology, and Astrophysics, and the network of U.S. movie actors. These networks are all bipartite: the collaborators (scientists, actors) and the collaborations (publications, movies) can be represented by two different kinds of vertices, and the links in the system are
FIG. 2. $\phi(k)$ obtained from the restructuring data of the MC simulation with $C_1 k$ subtracted, together with fits. For the case of $E=0$ (random rewiring, circles), the system converges to a classical random graph, which results in a narrow degree distribution. In the system with $E=-k \ln(k)$ (crosses), the interval in which $\phi(k)$ can be obtained is wider. Thus the results from reverse engineering are in good agreement with the initial MC energies.

always placed between vertices of different types (a scientist is connected to the papers in which he/she is a coauthor). Unipartite projections of these graphs can be made by keeping only one kind of the vertices and placing a link between them if they are linked to a common vertex of the other type in the bipartite graph. In the cases studied in this paper, the projection onto the graphs of collaborators has been used: the nodes represent collaborators (scientists or movie actors) and two nodes are linked if they have a common collaboration (articles, movies). In the graphs obtained this way, both edges and vertices are distinguishable and multiple links between vertices are allowed.

The collaboration network databases we have used [22,23] provide the time of the emergence of the links, but the times when they disappear are not defined. In other words, the time we consider an edge to be alive after its birth influences the structure of the graphs representing the system year after year. This parameter will be denoted by $\tau$, the lifetime of an edge. The minimal value for $\tau$ is equal to the time resolution of the data set. In case of $\tau=\infty$, the system is simply growing and no edges are deleted. Evidently, the choice of $\tau$ may influence all statistical properties of the network.

The number of vertices in these systems is changing slowly with time, but the number of edge restructuring events per time step is larger by two orders of magnitude than the change in the number of vertices. Therefore, the effect of the increase or decrease in $N$ can be neglected, and we use the time average of the right hand side of Eq. (12) (derived for a fixed $N$) to calculate $\phi(k)$.

The most important statistical properties of the studied networks are summarized in Table I.

I. Neuroscience and math publications

Data on these two systems were obtained from Ref. [22]. The time resolution of the appearance of the new articles was one year in the data set. The upper boundary of the interval of $k$ taken into account in the reverse engineering was in the range of 20–40. The results in case of the neuroscience papers for $\tau=3$ yr are shown in Fig. 3, and very similar plots

<table>
<thead>
<tr>
<th>Time span</th>
<th>Time step</th>
<th>$\tau=1$ yr</th>
<th>$\tau=2$ yr</th>
<th>$\tau=3$ yr</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\langle N \rangle$</td>
<td>$\langle k \rangle$</td>
<td>$k_{\text{max}}$</td>
</tr>
<tr>
<td>Movie actors</td>
<td>1986–1999</td>
<td>1 yr</td>
<td>9223</td>
<td>28.04</td>
</tr>
<tr>
<td>Neurosci. publ.</td>
<td>1991–1998</td>
<td>1 yr</td>
<td>55057</td>
<td>7.837</td>
</tr>
<tr>
<td>Math publ.</td>
<td>1991–1999</td>
<td>1 yr</td>
<td>17279</td>
<td>2.737</td>
</tr>
<tr>
<td>hep-ph</td>
<td>1992–04.02</td>
<td>1 month</td>
<td>3202</td>
<td>7.14</td>
</tr>
<tr>
<td>astro-ph</td>
<td>1992–04.02</td>
<td>1 month</td>
<td>5472</td>
<td>10.90</td>
</tr>
<tr>
<td>cond-mat</td>
<td>1992–04.02</td>
<td>1 month</td>
<td>5648</td>
<td>4.16</td>
</tr>
</tbody>
</table>
were obtained for the math publications. In both cases, $\phi^*(k)$ and $\gamma^*(k)$ can be fitted with

$$
\phi^*(k) = -\tilde{a} k \ln(k), \quad \gamma^*(k) = -\tilde{a} \ln(k),
$$

where $\tilde{a}$ is a positive constant. The actual value of this constant was $\tilde{a}=0.96$ for the neuroscience publications and $\tilde{a}=0.99$ in the case of the math papers.

In both cases, $\phi(k=0)$ is separated from the $k \geq 1$ part by a gap, indicating that zero connection is unfavorable for the vertices. This is consistent with the observed degree distributions, in which the vertices of zero degree were suppressed. (In the case of the math papers, vertices with zero degree were totally absent.)

For $\tau=1$ and $\tau=2$, similar results can be obtained with modified fitting parameters.

2. The Los Alamos e-print archives

We also studied the restructuring of the coauthorship networks of three e-print archives: Condensed Matter, High Energy Physics—Phenomenology, and Astrophysics [23]. In all three cases, the time resolution of the appearance of the new manuscripts was one month. To be able to compare the properties of these systems to the previously investigated coauthorship networks, we set $\tau=1,2,3$ yr in these cases as well. From the point of view of the energy, the obtained behavior was very similar to the previous cases. For the Condensed Matter and High Energy Physics—Phenomenology networks, $k_{\text{max}}$ was in the range of that seen for the neuroscience publications, and for the Astrophysics archive it was somewhat larger ($k_{\text{max}}=80$). The nonlinear part of the empirical energies could be fitted with functions of the form given in Eq. (17). The value of the parameter $\tilde{a}$ in case of $\tau=3$ yr was $\tilde{a}=1.05$, $\tilde{a}=0.77$, $\tilde{a}=0.59$ for the Condensed Matter, High Energy Physics—Phenomenology, and Astrophysics archives, respectively.

The results for the Astrophysics archive are shown in Fig. 4. The gap at $k=0$ in the energy together with the suppression of the vertices with zero degrees seen in the case of the neuroscience and math publications is also present in all three systems.

3. The network of movie actors

In the data of the U.S. movie actor network [22], the time resolution of the appearance of new films was 1 yr. For this network, the allowed $k$ interval in the reverse engineering is reasonably wide. Similarly to the coauthorship networks studied in the previous paragraphs, the nonlinear part of the empirical energy can be fitted with functions of the form given in Eq. (17), and a gap at $k=0$ together with the suppression of the vertices with zero degrees can be observed. Our results for $\tau=3$ yr are shown in Fig. 5 with $\tilde{a}=0.74$.

C. Asset graphs of the New York Stock Exchange

In this study, we used the asset graph sequence received from [24]. These graphs were constructed from correlations of the 477 New York Stock Exchange (NYSE) traded stocks: in a given time window the 476 most strongly correlated pairs of papers were linked [20]. Therefore in this case the obtained graphs were simple graphs. The market data was recorded with a time window width of 1000 days, from 2 January 1980 to 31 December 1999, and the window was stepped monthly. This resulted in 195 time windows. In this case, the general rule used to determine $k_{\text{max}}$ would result in accepting such degrees also that are represented by less than one vertex on average, therefore $k_{\text{max}}$ was set equal to the highest degree represented by at least one vertex on average, yielding $k_{\text{max}}=20$.

Similarly to the collaboration networks, the nonlinear part of the empirical energy can be fitted using Eq. (17) with $\tilde{a}=1.7$, as shown in Fig. 6. For this system, the gap in the energy at $k=0$ seen in the case of the collaboration networks is absent, and accordingly the $C_0$ fitting parameter can be set to zero.
VI. DISCUSSION

For each studied natural network, the nonlinear part of the empirical single-vertex energy can be fitted with the same universal function given in Eq. (17). We note that (due to the relatively narrow intervals in $k$) power laws of the form $E = -B \Sigma_i k_i^d$ can be used for fitting equally well, with fitting parameters $B$ and $\beta$. However, the following two reasons make the logarithmic fit $E = -\tilde{\alpha} \Sigma_i \ln(k_i)$ far more favorable: first, this latter has fewer fitting parameters; and second, since in each example $\tilde{\alpha}$ has been found to be very close to unity (within a factor of 2), even $\tilde{\alpha}$ is not a real fitting parameter.

The logarithmic fit is also consistent with the rule of preferential attachment observed in growing networks [16,25,26]. This can be shown by estimating the energy change of a vertex by the derivative of $\phi^*(k) + \tilde{\alpha} k = -\tilde{\alpha} k \ln(k)$, yielding $\Delta E/T = -\tilde{\alpha} \ln(k)$ [the irrelevant linear term $\tilde{\alpha} k$ has been added to $\phi^*(k)$ for simplicity]. Plugging this into the Boltzmann factor $\exp[-\Delta E/T]$, the resulting acceptance/rejection ratio for a randomly selected move is proportional to $k^\alpha$. In the case of $\tilde{\alpha} = 1$ we recover the linear preferential attachment rule. For several growing networks, however, the preferential attachment was found to scale as $k^\alpha$ [16,26]. The values for $\alpha$ measured by Jeong et al. 16 are close to those we obtained for $\tilde{\alpha}$. Hence our results provide another justification of the preferential attachment rule.

Furthermore, in the second representation of the energy, in which vertices contribute to the total energy depending on the degrees of their neighbors, the energy contribution of vertex $i$ becomes $\gamma(i) = -\tilde{\alpha} \Sigma_{j \neq i} \ln(k_j)$, where $j$ runs over the neighbors of vertex $i$. This can be interpreted as follows: the vertices “feel” advantages in being linked to other vertices of high degree; hence the magnitude of a neighbor’s contribution to the energy of vertex $i$ is a monotonically increasing function of that neighbor’s degree. The distinction between the neighbors in this picture follows the general Weber-Fechner law of sensation: a stimulus of a given degree generates a perception proportional to the logarithm of that degree in the neighbors. This logarithmic law of perception is natural in cases where the intensity of the stimulus may vary over several orders of magnitude, which is the case for degrees in scale-free networks.

Another situation where the use of $g(k)$ is very convenient is when it is advantageous to reach many other vertices via short paths, but it is expensive to have lots of connections. Under such circumstances the best strategy is to connect to a few other vertices with high degrees: numerous vertices can be reached in two steps at the cost of few own links. If the number of total edges is allowed to vary, such a scenario could simply be modeled by a decreasing $g(k)$ function [such as $-\ln(k)$] together with a negative chemical potential (corresponding to a linear penalty for the own links of a vertex).

VII. SUMMARY

We developed a reverse engineering method to deduce the preferences governing the restructuring in nongrowing networks from the statistics of the observed relocations. Our approach is applicable to systems where the preferences can be interpreted by single-vertex energy functions and the dynamics obeys detailed balance. The method was first tested on Monte Carlo simulations run with known energy functions, yielding reassuring results. Real networks such as the coauthorship network of scientific publications, the network of U.S. movie actors, and the asset graphs of the New York Stock Exchange were also studied.

In each case, the nonlinear part of the single-vertex energy function could be fitted with the same universal function $E = -\tilde{\alpha} \Sigma_i \ln(k_i)$ with $0.5 < \tilde{\alpha} < 2$. This energy is shown to be consistent with the preferential attachment rule of growing networks.

Furthermore, the obtained energy can be alternatively written as $E = -\tilde{\alpha} \Sigma_i \ln(k_i)$, where the summation for $i'$ runs over the neighbors of vertex $i$. In this representation the energy contributions of the vertices can be interpreted by the general Weber-Fechner law of sensation: the stimulus of a given vertex generates a perception in its neighbor proportional to the logarithm of that degree.

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[22] The data were downloaded from the following database, provided by Hawoong Jeong: http://www.nd.edu/~networks/database/index.html
[23] The coauthorship data were kindly provided by Simeon Warner (private communications).
[24] The asset graph sequence was kindly provided by J.-P. Onnela and J. Kertész (private communications).