Homogeneous complex networks

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We discuss various ensembles of homogeneous complex networks and a Monte-Carlo method of generating graphs from these ensembles. The method is quite general and can be applied to simulate micro-canonical, canonical or grand-canonical ensembles for systems with various statistical weights. It can be used to construct homogeneous networks with desired properties, or to construct a non-trivial scoring function for problems of advanced motif searching.

I. INTRODUCTION

Complex networks is a new emerging branch of random graph theory. For a long time random graphs have been mainly studied by pure mathematics but recently due to the availability of empirical data on real-world networks they have attracted the attention of physics and natural sciences (see for review [1, 2, 3]). Methods of statistical physics, both empirical and theoretical, have thus begun to play an important role in this research area.

The empirical observations of real-networks has had a feedback on theoretical development which now concentrated on the understanding of the observed features. For example fat tails in node degree distribution, small world effect, degree-degree correlations, or high clustering. Two complementary approaches have been developed: diachronic, known as growing networks [1, 2, 3], and synchronic being a sort of statistical mechanics of networks [4, 5, 6, 7, 8, 9].

We will discuss here the latter. This approach is a natural extension of Erdős and Rényi ideas [10, 11]. It is well suited both for growing (causal) networks for which nodes’ labels reflect the causal order of nodes’ attachment to the network [12, 13] and for homogeneous networks for which nodes’ labels can be permuted freely in an arbitrary way. Here we shall discuss mainly homogeneous networks. We shall shortly comment on causal networks towards the end of the paper.

The main aim of the paper is to present a consistent picture of statistical mechanics of networks. Some ideas have already been introduced earlier. They are scattered in many papers and discussed in many different contexts. We put them together, add some new material and introduce a guideline to obtain a self-contained introduction to statistical mechanics of complex networks.

The basic concept in the statistical formulation is statistical ensemble. Statistical ensemble of networks is defined by ascribing a statistical weight to every graph in the given set [4, 5]. Physical quantities are measured as weighted averages over all graphs in the ensemble. The probability of the occurrence of a graph in random sampling is proportional to its statistical weight. If the statistical weight changes then also the probability of occurrence of randomly sampled graphs will change and in effect different random graphs will be observed. The concept of statistical weight is crucial, since it defines randomness in the system. Statistical weight is built out of two ingredients: configuration space weight and functional weight. The configuration space weight is proportional to the uniform probability measure on the configuration space which tells us how to uniformly choose graphs in the configuration space. To illustrate the meaning of the uniform measure consider an ensemble of Erdős-Rényi graphs with \( N \) nodes and \( L \) links [14, 15]. The configuration space consists of \( \binom{N}{2} \) graphs with labeled nodes. All those graphs are equiprobable, and therefore the configuration space weight is the same for each graph. It is convenient to choose this weight to be \( 1/N! \) since then it can be interpreted as a factor which takes care of \( N! \) possible permutations of nodes’ labels. This factor has the same origin as the corresponding factor in quantum mechanics for indistinguishable particles and it is constant for all graphs in a finite \( N \)-ensemble.

We can calculate the entropy of random graphs as

\[
S = \ln \frac{1}{N!} \binom{N}{2}.
\]

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In the limit of large sparse graphs: $N \to \infty$ and $\frac{2L}{N} = \alpha = \text{const} > 2$, the entropy is an over-extensive function of the system size:

$$S = \frac{\alpha - 2}{2} N \ln N + \ldots,$$

unlike in standard thermodynamics.

Let us move to weighted graphs. The idea is to modify the Erdős-Rényi ensemble by introducing a functional weight which explicitly depends on graph’s topology. For example, if we choose the functional weight to be a function of the number of loops on the graph, we can suppress of favor loops of typical graphs in the ensemble. In a similar way we can choose statistical weights to control the node degree distribution to produce homogeneous scale-free graphs or to introduce correlations between degrees of neighboring nodes [15, 16, 17, 18].

Classical thermodynamics describes systems in equilibrium for which the functional weight is given by the Gibbs measure: $\sim \exp(-\beta E)$, where $E$ is the energy of the system. When discussing complex networks it is convenient to abandon the concept of energy and Gibbs measure and consider a more general form of statistical weights because many networks are not in equilibrium. Indeed, many networks emerging as a result of a dynamical process like growth are far from equilibrium [1, 2, 3]. It does not mean though that one cannot introduce a statistical ensemble of growing networks. On the contrary, one can for example consider an ensemble of networks which result of many independent repetitions of the growth process terminated when the network reaches a certain size. Such a collection of networks does not describe a thermodynamic equilibrium. The functional weight can be deduced from the parameters of the growth process but of course it has nothing to do with the Gibbs measure.

In fact, many real-world networks result from a combination of a growth process and some thermalization processes. For example, the Internet grows but at the same time it continuously rearranges. The latter process introduces a sort of thermalization. Today the growth has probably still larger influence on the topology of the underlying network but in the future the growth may slow down due to saturation and then equilibration processes resulting from continuous rewirings will take over. Similarly all evolutionary networks emerge from a growth mixed with a sort of thermalization related to the continuous network rearrangement. Therefore it is convenient to have a formalism which can extrapolate between the two regimes in a flexible way. The approach which we propose here is capable of modeling functional properties of networks by choosing an appropriate functional weight.

Let us return to the configuration space weight. As we mentioned this weight is equivalent to the uniform probability measure on the configuration space for which all graphs are equiprobable. It is a very crucial part of the construction of the ensemble to carefully specify what one means by equiprobable graphs. Consider first graphs with $N$ nodes. There are at least two natural candidates for the uniform measure in such a set of graphs. Since one is interested in shape (topology) of graphs one can define all shapes to be equiprobable. Alternatively one can introduce labels for nodes of each graph to obtain a set of labeled graphs and then one can define all labeled graphs to be equiprobable. The two definitions give two different probability measures since the number of ways in which one can label graph nodes depends on graph’s topology and thus the probability of occurrence of a given graph will depend on its topology too. It turns out that the latter definition is more natural. As we have seen above this definition leads to Erdős-Rényi graphs. So we stick to this definition and from here on we shall ascribe to each labeled graph the configuration space weight $1/N!$ which is constant in the set of graphs of size $N$.

The situation is more complex if one considers pseudographs that is graphs which have multiple connections (more than one link between two nodes) or self-connections (a link having the same node at its endpoints). In this case one can also label links and ascribe the same statistical weight to each fully labeled graph. For this choice the statistical weight of each graph is equal to the symmetry factor of Feynman diagrams generated in the Gaussian perturbation field theory [1].

The paper is organized as follows. In the next section we will recall some basic definitions. Then we will discuss Erdős-Rényi graphs in the context of constructing statistical ensemble and later we will generalize the construction to weighted homogeneous graphs. After this we will describe Monte-Carlo algorithms to generate graphs for canonical, grand-canonical and micro-canonical ensembles and discuss their representation in terms of adjacency matrices. A section will be devoted to pseudographs. In the last section we will shortly summarize the paper.

### II. DEFINITIONS

Let us first introduce some terminology. Graph is a set of $N$ nodes (vertices) connected by $L$ edges (links). A graph need not be connected. It may have many disconnected components including empty nodes (without any link). If a graph has no multiple or self-connected links we shall call it simple graph or graph. An example is illustrated in Fig. 1. Later we shall also discuss graphs with multiple- and self-connections. To distinguish them from simple graphs we shall call them degenerate graphs or pseudographs. One can consider directed or undirected graphs. Directed graphs...
FIG. 1: An example of simple graph with \( N = 6, L = 5 \). Vertices without links (like no. 2) are allowed. Each vertex can have at most \( N - 1 \) links. Positions of vertices in the picture are meaningless. The only information which matters is connectivity.

are built of directed links while undirected of undirected ones. In this paper we shall discuss undirected graphs but the discussion can easily be generalized to directed ones as well. Sometimes we will find it convenient to represent an undirected link as two oriented links going in opposite directions.

A simple graph can be represented by its adjacency matrix which is an \( N \times N \) matrix whose entries \( A_{ij} \) are equal to one if there is a link between vertices \( i, j \) or zero otherwise. Since self-connections are forbidden we have \( A_{ii} = 0 \) on the diagonal. The adjacency matrix of an undirected graph is also symmetric because if there is a link \( i \rightarrow j \) \((A_{ij} = 1)\), there must be also the opposite one \( j \rightarrow i \) \((A_{ji} = 1)\).

In this paper we want to construct statistical ensembles of homogeneous graphs having desired properties. We discuss three types of ensembles: ensemble of graphs with a fixed number of nodes \( N \) and varying number of links, ensemble with a fixed number of nodes \( N \) and a fixed number of links \( L \), and finally ensemble of graphs with a given node degree sequence \( \{q_1, q_2, \ldots, q_N\} \), which we shall call grand-canonical, canonical and micro-canonical ensembles, respectively. There are of course many other possibilities like for instance ensembles with varying number of nodes, or with a fixed number of loops etc, but the three mentioned above are encountered most frequently. To construct a statistical ensemble, for the chosen set of graphs, we have to specify statistical weight for each graph in the considered set.

In the next section using the Erdős-Rényi graphs and binomial graphs we will deduce a general logical structure standing behind the construction of ensembles of homogeneous graphs and then we will use this structure to introduce ensembles with an arbitrary functional weight which explicitly depends on the node degrees.

III. STATISTICAL ENSEMBLE FOR ERDŐS-RÉNYI RANDOM GRAPHS

For simplicity, we start from a well-known model of Erdős-Rényi’s graphs [10, 11]. In this classical model one considers simple graphs with \( N \) labeled nodes and \( L \) links [32] chosen at random out of all \( \binom{N}{2} \) possibilities. All possibilities are equiprobable and so are the corresponding graphs – understood as graphs whose vertices are labeled. Usually one is interested in unlabeled graphs that is in their shape or topology and not in their labeled version. To explain what is meant by graph’s shape or topology, let us consider a simple graph shown in the upper part of Fig. 2. Unlabeled graph (topology) on the left hand side of the figure is represented as labeled graphs on the right hand side. There are six possible realizations, but only three of them: \( A, C, E \) are distinct. \( B \) is the same as \( A \) since it can be obtained from \( A \) by a continuous deformation: one can continuously move the vertex 2, together with the link

![Graphs](image-url)
Attended to it, to the position of the vertex 3, and at the same time the vertex 3 to the position of the vertex 2. Such a continuous deformation does not change graph’s connectivity. The same holds for pairs: C, D and E, F. This can also be seen if we take into account the adjacency matrix \( A \). Both A and B have identical adjacency matrices which are different from those for C, D and E, F:

\[
A_A = A_B = \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 0 \\
1 & 0 & 0
\end{pmatrix}, \quad A_C = A_D = \begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix}, \quad A_E = A_F = \begin{pmatrix}
0 & 0 & 1 \\
0 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}.
\]

Now we remove labels from all graphs in Fig. 2 to obtain two unlabeled graphs depicted on the left hand side. Although there are three distinct adjacency matrices for the upper shape, all of them lead to the same connections between vertices (unlabeled graph). The graph in the lower line in Fig. 2 can be labeled only in one way\(^\text{[33]}\) which is represented by the following adjacency matrix:

\[
A_G = \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}.
\]

Thus the triangular shape has only one realization as labeled graph. Furthermore, the upper and lower graphs are obviously distinct because none of the corresponding labeled graphs (adjacency matrices) representing the upper graph is equal to that for the lower graph. In this trivial case the difference is in the number of links. More generally, any two graphs are distinct if the underlying labeled graphs (adjacency matrices) cannot be converted one into another by a permutation of nodes’ labels. It is clear that for the graphs in Fig. 2 there is no such a permutation but in general case the comparison of graphs may be a complex problem.

Let us now apply the ideas sketched above to define an ensemble of graphs. As an example we shall consider\(^\text{[34]}\) Erdős-Rényi graphs with \( N = 4, L = 3 \). It consists of three distinct graphs A, B, C shown in Fig. 3. Now we want to determine the statistical weight for those graphs. Adjacency matrices of the underlying labeled graphs are essentially different for A, B, C since they cannot be converted one into another by a permutation of node’s labels. Each graph in Fig. 3 has a few possible realizations as labeled graph. One can label four vertices in \( 4! = 24 \) ways corresponding to permutations of 1 − 2 − 3 − 4 gives an identical labeled graph (adjacency matrix) as 4 − 3 − 2 − 1. The same kind of symmetry applies for remaining pairs of permutations. Therefore there are \( n_A = 12 \) labeled graphs for A. Similarly one can find that there are \( n_B = 4 \) labeled graphs for B and \( n_C = 4 \) for C. Altogether, there are \( n_A + n_B + n_C = 20 \) labeled graphs in accordance with \( n = \binom{N}{L} = 20 \). In the Erdős-Rényi ensemble labeled graphs are equiprobable, so the shapes A, B, C have the following probabilities:

\[
p_A = \frac{n_A}{n} = \frac{3}{5}, \quad p_B = \frac{n_B}{n} = \frac{1}{5}, \quad p_C = \frac{n_C}{n} = \frac{1}{5}.
\]

These probabilities give frequencies of the occurrence of the shapes A, B, C in random sampling. We see that graphs (unlabeled graphs) are not equiprobable in Erdős-Rényi’s ensembles.

Let us denote the statistical weights for A, B, C by \( w_A, w_B, w_C \) which are proportional to probabilities of configurations in the ensemble. In our case \( w_A : w_B : w_C = p_A : p_B : p_C \). There is a common proportionality constant in the weights. It is convenient to choose this constant in such a way that the weight of each labeled graph be \( 1/N! \).\(^\text{[34]}\) For this choice we have

\[
w_A = 1/2, \quad w_B = 1/6, \quad w_C = 1/6,
\]

for the graphs in Fig. 3. This choice compensates for the increasing factor of permutations \( N! \), when one considers ensembles with varying \( N \), and intuitively removes overcounting coming from summing over permutations of indistinguishable node’s labels. However, one should remember that in general the number of distinct labeled graphs of
a graph is less than $N!$ and therefore the weight of graph is smaller than 1. The larger is the symmetry of a graph topology the smaller is the number of underlying labeled graphs and thus the smaller is the statistical weight (see for instance Fig. 2).

The partition function $Z(N, L)$ for the Erdős-Rényi ensemble can be written in the form:

$$Z(N, L) = \sum_{\alpha' \in g(N, L)} \frac{1}{N!} = \sum_{\alpha \in g(N, L)} w(\alpha),$$

(7)

where $g(N, L)$ is the set of all labeled graphs with given $N, L$ and $g(N, L)$ is the corresponding set of (unlabeled) graphs. The weight $w(\alpha) = n(\alpha)/N!$, where $n(\alpha)$ is the number of labeled graphs of graph $\alpha$. We are interested in quantities averaged over the ensemble. More precisely, we are interested in quantities which depend on topology of graph and not on node’s labels. This means that if $O(\alpha)$ is such an observable then for any two labeled graphs $\alpha'_1$ and $\alpha'_2$ of graph $\alpha$ we have $O(\alpha'_1) = O(\alpha'_2) \equiv O(\alpha)$. The average is defined by

$$\langle O \rangle = \frac{1}{Z(N, L)} \sum_{\alpha' \in g(N, L)} O(\alpha') \frac{1}{N!} = \frac{1}{Z(N, L)} \sum_{\alpha \in g(N, L)} w(\alpha) O(\alpha).$$

(8)

We shall refer to an ensemble with fixed $N, L$ as to a canonical ensemble. The word ”canonical” is used here to emphasize that the number of links $L$ is conserved like the total number of particles in a container with ideal gas remaining in thermal balance with a source of heat. The partition function $Z(N, L)$ can be calculated by pure combinatorics as we have seen in the introduction. Now for completeness we derive it using the adjacency matrix representation of graphs. The adjacency matrices $A$ are symmetric, they have zeros on the diagonal and units above the diagonal. Thus we have

$$Z(N, L) = \sum_{A_{12} A_{13} \cdots A_{N1} A_{N2} \cdots} \sum_{A_{N-1,N}} \delta \left[ L - \sum_{p<r} A_{pr} \right] 1/N!,$$

(9)

where $\delta [x] = 1$ if $x = 0$ and zero elsewhere. The sums are done over all $A_{ij} = 0, 1$ for all pairs $i, j: 1 \leq i < j \leq N$. Using an integral representation of $\delta [x]$ and exchanging the order of summation and integration we obtain the expected result:

$$Z(N, L) = (1/N!) \frac{1}{2\pi} \int_{-\pi}^{+\pi} dk \ e^{ikL} \ (1 + e^{-ik})^{\binom{N}{2}} = (1/N!) \frac{1}{2\pi} \int_{-\pi}^{+\pi} dk \ e^{ikL} \ \sum_{m=0}^{\binom{N}{2}} \binom{\binom{N}{2}}{m} e^{-ikm}$$

$$= (1/N!) \left( \binom{\binom{N}{2}}{L} \right).$$

(10)

This method can be applied to calculate averages of various quantities. As an example consider the node degree distribution $\pi(q)$ which tells us what is the probability that a randomly chosen vertex on random graph has degree $q$:

$$\pi(q) = \left\langle \frac{1}{N} \sum_{i} \delta [q - q_i] \right\rangle.$$

(11)

By random graph we mean that we average over graphs from the given ensemble. We know that for Erdős-Rényi graphs $\pi(q)$ is a Poissonian distribution in the limit of $N \to \infty$:

$$\pi(q) = \frac{\bar{q}^q}{q!} \exp(-\bar{q}),$$

(12)

where $\bar{q} = 2L/N$ is the average vertex degree. This result can be rederived using the method described above. Let us look at the degree of a vertex labeled by one. The result does not depend on the vertex label for homogeneous graphs since labels have no physical meaning. One can find that

$$\pi(q) = \frac{1}{Z(N, L) N!} \sum_{A_{12} A_{13} \cdots A_{N-1,N}} \delta \left[ L - \sum_{p<r} A_{pr} \right] \delta \left[ q - \sum_{r=2}^{N} A_{1r} \right]$$

$$= \left( \frac{\binom{N}{2}}{L-q} \right) \left( \frac{N-1}{q} \right) / \left( \binom{\binom{N}{2}}{L} \right).$$

(13)
which in the limit $\tilde{q} = \text{const}$, $N \to \infty$ gives Eq. 12 as expected.

So far we have discussed the canonical ensemble of Erdős-Rényi graphs with $N, L$ fixed. Erdős and Rényi introduced also a related model called \textit{binomial model} where the number of nodes $N$ is fixed but the number of links $L$ is not fixed \textit{a priori}. One starts from $N$ empty vertices and connects every pair of vertices with a probability $p$. In this statistical ensemble the probability of obtaining a labeled graph with given $L$ is $P(L) = p^L(1 - p)^{(\tilde{N} - 2)}$. Thus the partition function is

$$Z(N, \mu) = \sum_{L} \sum_{\alpha \in g(N,L)} \frac{1}{N!} P(L(\alpha)) = (1 - p)^{(\tilde{N} - 2)} \sum_{L} \left( \frac{p}{1 - p} \right)^L \sum_{\alpha \in g(N,L)} \frac{1}{N!}$$

$$\propto \sum_{L} \exp(-\mu L) Z(N, L) \propto \sum_{L} \exp(-\mu L + S(N, L)), \quad (14)$$

where $\frac{p}{1 - p} = \exp(-\mu)$ or $\mu = \ln \frac{1 - p}{p}$, and the entropy $S(N, L)$ is given by Eq. 11. We skipped an $L$-independent factor in front of the sum in the second line substituting equality by proportionality sign. The weight of labeled graphs is $w(\alpha) = 1/N! \exp(-\mu L(\alpha))$, where $\mu$ is a constant which can be interpreted as chemical potential for links in the \textit{grand-canonical} ensemble 14. One can calculate the average number of links or its variance as derivatives of the grand-canonical partition function with respect to $\mu$: $\langle L \rangle = -\partial_{\mu} \ln Z(N, \mu)$ and $\langle L^2 \rangle - \langle L \rangle^2 = \partial_{\mu}^2 \ln Z(N, \mu)$. The sum of states can be done exactly:

$$Z(N, \mu) = \sum_{L=0}^{(\tilde{N})} e^{-\mu L} \frac{1}{N!} \left( \frac{N}{L} \right) = \frac{1}{N!} (1 + e^{-\mu})^{(\tilde{N})}, \quad (15)$$

It is easy to see that for fixed finite $\mu$ the average number of links behaves as $N^2$ or more precisely as

$$\langle L \rangle = \frac{p N(N - 1)}{2} = \frac{1}{1 + e^{\mu}} \frac{N(N - 1)}{2}. \quad (16)$$

Thus for $N \to \infty$ the graphs become dense. The mean value of node degree $\langle \tilde{q} \rangle = 2 \langle L \rangle / N$ increases to infinity. The situation changes when $\mu$ goes to infinity with increasing $N$. This happens in particular if the probability $p$ scales as $p \sim 1/N$ since then $\mu$ behaves as $\mu \sim \ln N$. In this case $L$ is proportional to $N$ 10 and both the terms $\mu L$ and $S$ in the exponent of Eq. 14 behave as $N \ln N$ and compensate each other. The corresponding graphs become sparse and the mean node degree $\langle \tilde{q} \rangle = 2 \langle L \rangle / N$ is now finite. The situation in which $\mu$ scales as $\ln N$ is very different from the situation known from classical statistical physics, where such quantities like chemical potential $\mu$ are intensive and do not depend on system size $N$ in the thermodynamic limit $N \to \infty$.

The difference between canonical and grand-canonical ensembles gradually disappears in the large $N$ limit 4, 8. For canonical ensemble or sparse graphs the node degree $\tilde{q} = 2L/N = \alpha$ is kept constant when $N \to \infty$ while in grand-canonical one it may fluctuate around the average $\langle \tilde{q} \rangle = 2 \langle L \rangle / N = \alpha$. However, the magnitude of fluctuations around the average disappears in the large $N$ limit since

$$\langle L^2 \rangle - \langle L \rangle^2 = \left( \frac{N}{2} \right) \frac{e^{-\mu}}{(1 + e^{-\mu})^2}, \quad (17)$$

and $\Delta q = \sqrt{\langle L^2 \rangle - \langle L \rangle^2} / \langle L \rangle \sim 1/N \to 0$, so effectively the system selects graphs with $\tilde{q} = \alpha$.

Sometimes one also considers an ensemble of graphs with a predefined node degree sequence $\{q_1, q_2, \ldots, q_N\}$. We shall call it \textit{micro-canonical}. Again, in the simplest case one assumes that all labeled graphs are equiprobable in this ensemble. Properties of random graphs in such an ensemble strongly depend on the degree sequence.

\section*{IV. WEIGHTED HOMOGENEOUS GRAPHS}

In the previous section we described ensembles for which all labeled graphs had the same statistical weight. Random graphs in such ensembles have well known properties. It turns out, however, that most of these properties do not correspond to those observed for real world networks. One needs a more general set-up to define an ensemble of complex random networks. Such a set-up can be introduced as follows. One considers the same set of graphs as in Erdős-Rényi model but one ascribes to each graph a different statistical weight. In other words, one chooses a probability measure on the set of graphs which differs from the uniform measure. In the generalized ensemble, each graph in addition to the configuration space weight $1/N!$ has a functional weight $W(\alpha)$. For homogeneous random graphs
Barabási - Albert distribution [19]:

\[ N \ln \text{canonical ensemble with } \pi \text{ obtain a desired form of the node degree distribution } q \text{ where } w(\alpha) = A \text{ random graphs with this node degree distribution. In this case the constants } \sum q \text{ chosen graph has degrees } \bar{q} \text{ weighted canonical ensemble reads} \]

\[ Z(N, L) = \sum_{\alpha' \in g(N, L)} (1/\alpha') W(\alpha') = \sum_{\alpha \in g(N, L)} w(\alpha) W(\alpha), \tag{18} \]

where \( w(\alpha) \) is the same factor \( w(\alpha) = n(\alpha)/N! \) as before [19], being just the ratio of the number of labeled graphs \( \alpha' \) of \( \alpha \) (obtained by permutations of nodes' labels giving distinct adjacency matrices) and the number of all nodes' labels permutations \( N! \). For Erdös-Rényi graphs the functional weight is \( W(\alpha) = 1 \).

The simplest non-trivial example is a family of product weights \( W \):

\[ W(\alpha) = \prod_{i=1}^{N} p(q_i), \tag{19} \]

where \( p(q) \) is a positive function depending on one node degree \( q \). This functional weight does not introduce correlations between node degrees. We shall refer to random graphs generated by this partition function as uncorrelated networks.

One should however remember that the total weight does not entirely factorize because the configuration space weight \( p(q) \) deviates from the limiting shape due to finite size corrections, which are particularly strong for fat tailed distributions.

For large \( N \), the node degree distribution \( \pi(q) \) [20], that is the probability that a random node on random graph has degree \( q \) [21, 22], can be approximated by

\[ \pi(q_1, \ldots, q_N) \sim \prod_{i=1}^{N} \pi(q_i). \tag{20} \]

For large \( L \), the node degree distribution \( \pi(q) \) [21], that is the probability that a random node on random graph has degree \( q \) [21, 22], can be determined from the conditions for the normalization \( \sum_q \pi(q) = 1 \) and for the average \( \sum_q q\pi(q) = \bar{q} = 2L/N \). For example, for \( p(q) = 1 \) which corresponds to Erdös-Rényi graphs one finds \( A = -\ln \bar{q} = \ln 2L/N \) and \( B = \bar{q} = 2L/N \), therefore \( \pi(q) \) is given by the Poissonian from Eq. [12].

Since the node degree distribution \( \pi(q) \) for weighted graphs [19] depends on \( p(q) \), one can choose the latter to obtain a desired form of the node degree distribution \( \pi(q) \). Let \( \pi(q) \) be a desired node degree distribution such that

\[ \sum_q \pi(q) = 1, \quad \bar{q} = \sum q\pi(q). \tag{22} \]

If we choose the weight [19] with

\[ p(q) = q! \pi(q) \tag{23} \]

in canonical ensemble with \( N \) nodes and \( L \) links, in the limit of \( N \to \infty \) and \( 2L/N = \bar{q} \) we obtain homogeneous random graphs with this node degree distribution. In this case the constants \( A, B \) from Eq. [21] vanish automatically: \( A = B = 0 \). In particular by an appropriate choice of \( p(q) \) we can generate scale free graphs with the node degree Barabási - Albert distribution [19]; \( \pi(q) = 4/(q(q+1)(q+2)) \) for \( q = 1, 2, \ldots \) and \( \pi(0) = 0 \) as an ensemble of graphs \( L = N, \bar{q} = 2 \) with \( p(q) = q!/q(q+1)(q+2) \) for \( q = 1, 2, \ldots \) and \( p(0) = 0 \). However, for finite \( N \) the node degree distribution \( \pi(q) \) deviates from the limiting shape due to finite size corrections, which are particularly strong for fat tailed distributions \( \pi(q) \sim q^{-\gamma} \). The maximal node degree scales as \( q_{\text{max}} \sim N^{1/(\gamma-1)} \) for \( \gamma \geq 3 \) and as \( q_{\text{max}} \sim N^{1/2} \) for very fat tails: \( 2 < \gamma < 3 \) [14, 20] as a result of structural constraints which also lead to the occurrence of correlations between node degrees.

One can define more complicated weights than those given by Eq. [19]. A natural candidate for networks with degree-degree correlations is the following weight [2, 13]:

\[ W(\alpha) = \prod_{i=1}^{L} p(q_{a_i}, q_{b_i}). \tag{24} \]
where the product runs over all links of the graph, and the weight \( p(q_a, q_b) \) is a symmetric function of degrees of nodes at the end points of the link. One can choose this function to favor assertive or disassertive behavior \( E \Rightarrow E \Rightarrow E \Rightarrow E \Rightarrow E \). In a similar way one can introduce probability measures on the set of graphs which mimic some other functional properties of real networks, like for example higher clustering [21, 22, 23, 24, 25]. One can do this in micro-canonical, canonical, grand-canonical or any other ensemble. This is just the most general set-up to handle homogeneous networks.

V. MONTE-CARLO GENERATOR OF HOMOGENEOUS NETWORKS

Erdős-Rényi graphs are exceptional in the sense that one can calculate for them almost all quantities of interest analytically. This is not the case for weighted networks. Various methods have been proposed for generating random graphs [26]. In this section we will describe a Monte-Carlo method which allows one to study a wide class of random weighted graphs experimentally by a sort of numerical experiments. The basic idea behind this type of experiments is to sample the configuration space of graphs with the probability proportional to the statistical weight or in other words to generate graphs with a desired probability. Again, the Erdős-Rényi graphs are exceptional because one can generate them one by one independently of each other. This is just because they are equiprobable. For weighted graphs the situation is not that easy since there are no efficient algorithms to pick up an element from a large set with the given probability. The naive algorithm which relies on picking up an element uniformly and then accepting it with the given probability has a very low acceptance rate. Therefore one has to use another idea. We will describe below how to generate graphs using dynamical Monte-Carlo technique.

The idea is to run a random walk process in the set of graphs which visits configurations with a frequency proportional to their statistical weight. Mathematically, this means that one has to invent a stationary Markov chain (process) for which the stationary distribution is proportional to the statistical weights of graphs: \( \sim W(\alpha)/Z \).

The Markov chain is defined by transition probabilities \( P(\alpha \to \beta) \) that the random walker will go in one step from a configuration (graph) \( \alpha \) to \( \beta \). The probabilities are stored in a transition matrix \( P \): \( P_{\alpha\beta} \equiv P(\alpha \to \beta) \) which is also called Markov’s matrix. For a stationary process, the transition matrix \( P \) is constant during the random walk. Random walk is initiated from a certain graph \( \alpha_0 \) and then elementary steps are repeated producing a sequence (chain) of graphs \( \alpha_0 \to \alpha_1 \to \alpha_2 \to \ldots \). The probability \( p_\beta(t+1) \) that a graph \( \beta \) will be generated in the \((t+1)\)-th step of the Markov process can be calculated as

\[
p_\beta(t+1) = \sum_\alpha p_\alpha(t) P_{\alpha\beta}.
\]

The last equation can be written as

\[
p(t+1) = P^T p(t),
\]

where \( \tau \) denotes transposition, and \( p \) is a vector of elements \( p_\alpha \). One should note that the stationary state: \( p(t+1) = p(t) \) corresponds to a left eigenvector of \( P \) to the eigenvalue \( \lambda = 1 \). If the process is ergodic, which means that any configuration can be reached by a sequence of transitions starting from any initial configuration, and if the transition matrix fulfills the detailed balance condition:

\[
W_\alpha P_{\alpha\beta} = W_\beta P_{\beta\alpha} \ \forall \alpha, \beta,
\]

then the stationary state can be shown to approach the desired distribution: \( p_\alpha(t) \to W_\alpha/Z \) for \( t \to \infty \). We used a short-hand notation \( W_\alpha \) for \( W(\alpha) \). In other words, when the length of the Markov chain becomes infinite the probability of occurrence of graphs in the Markov chain becomes proportional to their statistical weights and becomes independent of the initial configuration. Therefore the average over graphs generated in this Markovian random walk is a good estimator of the average over the weighted ensemble. The price to pay for generating graphs in this way is that the consecutive graphs in the Markov chain may be correlated with each other. Therefore one has to find a minimal number of steps for which one can treat measurements on such graphs as independent.

One should note that the only characteristics of the Markov process which has a physical meaning from the point of view of the simulated ensemble is the stationary distribution. All other dynamical properties of the random walk which are encoded in the form of transition matrix \( P(\alpha \to \beta) \) are irrelevant. Many different transition matrices \( P \) may have the same stationary distribution. Indeed, many of them fulfill the detailed balance condition for given weights \( W_\alpha \) [21]. The best known choice of \( P \) is

\[
P_{\alpha\beta} = \min \left\{ 1, \frac{W_\beta}{W_\alpha} \right\}.
\]
VI. MONTE-CARLO GENERATOR OF CANONICAL ENSEMBLE

Now, we want to apply this method to generate Erdős-Rényi graphs. Let us begin with the canonical ensemble with \( N, L \) fixed. A good candidate for elementary transformation of graph is rewiring of a link as shown in Fig. 4 because it does not change \( N \) and \( L \). As mentioned before it is convenient to introduce a representation in which each undirected link is represented by two directed links. The rewiring is done in two steps\[4\]. First we choose a directed link \( ij \) and a vertex \( k \) at random. Then we rewire the link \( ij \) to \( ik \). If there is already a link between \( i \) and \( k \) or if the vertex \( k \) coincides with \( i \), we reject the rewiring since it would otherwise lead to a multiple- or self-connection. One should note that the result of rewiring \( ij \) is not the same as of rewiring \( ji \). The move is accepted with the Metropolis probability\[28\].

![Fig. 4: The idea of rewiring](image)

Let us see how rewiring transformations work in practice. Consider as an example the set of graphs shown in Fig. 3. If we pick up the link \( 3 \rightarrow 2 \) in the graph A and rewire it to \( 3 \rightarrow 1 \), we will obtain the graph B. If we rewire the link \( 2 \rightarrow 3 \) to \( 2 \rightarrow 4 \), we will get the graph C. So using the procedure of rewiring showed in Fig. 4 we can obtain every graph in the ensemble. The rewiring transformation is ergodic in this set of graphs.

To summarize, our procedure of generating graphs in this training ensemble looks as follows. We construct an arbitrary graph having \( N = 4 \) nodes and \( L = 3 \) links to initiate the procedure and then we repeat iteratively rewirings for randomly chosen links and vertices. The only restriction is that the rewirings do not produce self- or multiple-connected links. We keep on repeating until we obtain "thermalized graphs". Then we can begin measuring quantities on the generated sequence of random graphs.

Let us check that the described Monte-Carlo procedure indeed generates graphs with the expected probabilities\[5\]. Let us calculate the Markovian matrix \( P \) for the rewiring procedure in this ensemble. First we calculate the transition probability from A to B. The graph A can be converted into B in one step if we rewire the link "$b" in Fig. 5 to the vertex 2, or alternatively the link "$c" to the vertex 1. We see that for this change we can choose two out of six links and one of four vertices to obtain the desired change. Thus the probability of choosing links is \( 2/6 \) and of choosing correct vertex is \( 1/4 \), so the total probability is \( P(A \rightarrow B) = 2/6 \cdot 1/4 = 2/24 \). Let us now calculate \( P(A \rightarrow C) \). To obtain C from A we have to rewire "$a" to 3 or "$f" to 4. Thus \( P(A \rightarrow C) = 2/6 \cdot 1/4 = 2/24 \). We can find \( P(A \rightarrow A) \) from the condition: \( P(A \rightarrow A) + P(A \rightarrow B) + P(A \rightarrow C) = 1 \). This yields \( P(A \rightarrow A) = 20/24 \).

Repeating the calculations for the remaining cases we find: \( P(B \rightarrow A) = 6/24, P(B \rightarrow B) = 18/24, P(B \rightarrow C) = 0 \) and \( P(C \rightarrow A) = 6/24, P(C \rightarrow B) = 0, P(C \rightarrow C) = 18/24 \). The results can be collected in a transition matrix:

\[
P = \frac{1}{24}\begin{bmatrix} 20 & 2 & 2 \\ 6 & 18 & 0 \\ 6 & 0 & 18 \end{bmatrix}.
\] (29)

We can now determine the stationary probability distribution of the Markov process as a left eigenvector to the eigenvalue one of the transition matrix \( P \). We obtain \( p_A : p_B : p_C = 3 : 1 : 1 \) in agreement with Eq.\[5\]. This is not surprising since \( P \) satisfies the detailed balance condition\[27\] and the corresponding changes are ergodic.
We have checked above by explicit calculation that the algorithm gives correct weights of Erdős-Rényi graphs for \( N = 3, L = 4 \). One can give a general argument that for any \( N, L \) the algorithm generates labeled graphs which are equiprobable. Suppose that we have a certain labeled graph \( \alpha \) and want to get \( \beta \) by rewiring \( ij \) to \( ik \). (see Fig. 4). The total probability \( P(\alpha \rightarrow \beta) \) can be written as a product of two factors: the probability \( P_{\alpha} \) of choosing a particular candidate for a new configuration and the probability \( P_{\beta} \) of accepting it. Because we choose a link \( i \rightarrow j \) from \( 2L \) possible directed links and a vertex \( k \) from \( N \) vertices we have \( P_{\beta} = 1/(2LN) \). Inserting \( P(\alpha' \rightarrow \beta') = 1/(2LN) P_{\alpha}(\alpha' \rightarrow \beta') \) in the Eq. \( (28) \) and similarly for \( \alpha' \leftrightarrow \beta' \) we get

\[
w_{\alpha'} P_{\alpha}(\alpha' \rightarrow \beta') = w_{\beta'} P_{\beta}(\beta' \rightarrow \alpha').
\]

But \( w_{\alpha'} = 1/N! \) for all labeled graphs, thus \( P_{\alpha}(\alpha' \rightarrow \beta') = P_{\beta}(\beta' \rightarrow \alpha') \). This means that every move should be accepted unless it violates the multiple- or self-connections constraints. The rejection does not change the frequency of the occurrence of simple graphs but only restricts the space of sampled graphs to what we need. The weights of (unlabeled) graphs \( \alpha \) are in this case \( w(\alpha) = n(\alpha)/N! \) where \( n(\alpha) \) is the number of distinct graphs of \( \alpha \).

| Graphs | \( w_{\alpha} \) | \( p_{\alpha} \) | \( w_{\alpha} \) | \( p_{\alpha} \) | \( w_{\alpha} \) | \( p_{\alpha} \) | \( w_{\alpha} \) | \( p_{\alpha} \) |
|--------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
|        | 1/2            | 0.286          | 1/12           | 0.048          | 1/2            | 0.286          | 1/8            | 0.071          |
|        | 0.286          | 0.286          | 0.048          | 0.286          | 0.071          | 0.286          | 0.024          | 0.024          |

| R      | 10  | 0.285(1) | 0.286(1) | 0.048(1) | 0.286(1) | 0.071(1) | 0.024(1) |
|--------|-----|----------|----------|----------|----------|----------|----------|
|        | 5   | 0.286(1) | 0.285(1) | 0.047(1) | 0.286(1) | 0.071(1) | 0.024(1) |
|        | 2   | 0.285(1) | 0.285(1) | 0.047(1) | 0.286(1) | 0.072(1) | 0.024(1) |
|        | 1   | 0.284(1) | 0.286(1) | 0.048(1) | 0.284(1) | 0.072(1) | 0.025(1) |

TABLE I: Theoretically calculated weights \( w_{\alpha} \) of graphs in the canonical ensemble \( N = 5, L = 4 \) are normalized to ensure probabilistic interpretation: \( p_{\alpha} = w_{\alpha} / \sum_{\beta} w_{\beta} \), and compared with the experimental frequencies in the Markov chain using algorithm of rewiring. The results differ by the number \( R \) of rewirings between consecutive measurements.

Let us numerically test the algorithm. In table \( \| \) we compare the weights calculated analytically and computed from Monte-Carlo generated graphs for \( N = 5, L = 4 \). There are six different graphs in this ensemble. We generated \( 10^6 \) graphs. Each of them was obtained from the previous one by \( R \) rewirings, or more precisely by \( R \) attempts of rewiring \( 36 \).

As we can see in table \( \| \) the frequency of occurrence of each graph is in an excellent agreement with the expected weights. The results do not depend on the separation \( R \) between the measurements. In the chain of \( 10^6 \) graphs, each graph in this ensemble is produced many times. For larger ensembles the algorithm would not be able to visit all graphs since the number of graphs is very large \( \| \). In this case the algorithm would choose only those graphs which are most representative. To make sure that the algorithm has reached the stationary distribution one should start a couple of random walks from different corners of the configuration space and run the algorithm so long as the statistical properties of graphs generated in all the random walks become identical.

Generalization of the algorithm to a weighted ensemble is straightforward. We insert the statistical weights \( W_{\alpha} \) of this ensemble into the Metropolis formula \( (28) \). Consider in particular a product weight \( (19) \). We choose a link \( ij \) and a vertex \( k \) on the current configuration \( \alpha \) at random and attempt to rewire the link to \( ik \) to obtain a new configuration \( \beta \). The change is accepted with the probability

\[
P_{\alpha}(\alpha \rightarrow \beta) = \min \left\{ 1, \frac{W_{\beta}}{W_{\alpha}} \right\} = \min \left\{ 1, \frac{p(q_j - 1)p(q_k + 1)}{p(q_j)p(q_k)} \right\}.
\]

FIG. 5: The representation of graph A in Fig. 3 as directed graph.
The move removing a link is done in a different way. Instead of picking up a link as a candidate, one could pick up a link-candidate for which the move is to be applied. It is convenient to split the total transition probability into three factors:

\[ P(\alpha \rightarrow \beta) = p_{\pm} P_c(\alpha \rightarrow \beta) P_{\alpha}(\alpha \rightarrow \beta), \]  

where \( p_\pm \) stands for one of \{\( p_- \), \( p_+ \)\}, \( P_c(\alpha \rightarrow \beta) \) for the probability of choosing a candidate configuration for the change and \( P_{\alpha}(\alpha \rightarrow \beta) \) for the probability of accepting the move. Let \( \alpha \) and \( \beta \) be two graphs which differ by a link which is present on \( \beta \) but absent on \( \alpha \): \( L(\alpha) = L(\beta) - 1 \). The transition probability for adding a link to \( \alpha \) has to be balanced with the probability of removing the link from \( \beta \). In order to add a link to \( \alpha \) we have to choose two vertices to which the addition of a link is attempted. The probability of choosing a given pair of vertices, if we choose two vertices independently, is \( P_c(\alpha \rightarrow \beta) = 2/N^2 \). Thus the total probability of this move is

\[ P_{\alpha\beta} = P(\alpha \rightarrow \beta) = p_+ \frac{2}{N^2} P_{\alpha}(\alpha \rightarrow \beta). \]  

In the reciprocal transformation we have to choose this link among all links. The probability of choosing one among \( L \) links is \( P_{c}(\beta \rightarrow \alpha) = 1/L_\beta = 1/(L_\alpha + 1) \). Thus the total probability of this move is

\[ P_{\beta\alpha} = P(\beta \rightarrow \alpha) = p_- \frac{1}{L_\beta} P_{\beta}(\beta \rightarrow \alpha). \]  

Now we have to insert the last two equations to the detailed balance condition which for the grand-canonical ensemble additionally includes the factor \( e^{-\mu L} \):

\[ W_\alpha e^{-\mu L_\alpha} P_{\alpha\beta} = W_\beta e^{-\mu L_\beta} P_{\beta\alpha}. \]  

Using this we can calculate the ratio

\[ \frac{P_{\alpha}(\alpha \rightarrow \beta)}{P_{\alpha}(\beta \rightarrow \alpha)} = \exp(-\mu) \frac{p_-}{p_+} \frac{N^2}{2L_\beta} W_\beta W_\alpha. \]  

If one chooses the same number of attempts for adding and removing a link: \( p_+ = p_- \), then the ratio \( p_+/p_- = 1 \) will disappear from the last equation and the acceptance probabilities for adding or removing a link in the Metropolis algorithm will read

\[ P_{\alpha}(\alpha \rightarrow \beta) = \min \left\{ 1, \exp(-\mu) \frac{N^2}{2(L_\alpha + 1)} \frac{W_\beta}{W_\alpha} \right\}, \]  

and

\[ P_{\alpha}(\beta \rightarrow \alpha) = \min \left\{ 1, \exp(+\mu) \frac{2L_\beta}{N^2} \frac{W_\alpha}{W_\beta} \right\}, \]  

respectively. As before if we want to produce only simple graphs we must have an additional condition which eliminates moves leading to self- or multiple connections. The algorithm is complete. One should note that there is no reason to do additional rewirings because a rewiring of a link \( ij \) to a link \( ik \) is equivalent to removing the link \( ij \) and adding \( ik \).

In principle one could propose other algorithms. For example, one could consider a modified algorithm in which the move removing a link is done in a different way. Instead of picking up a link as a candidate, one could pick up
two vertices at random, and then remove a link if there is any between them. The probability of choosing a pair of vertices would be $2/N^2$ and it would cancel with the identical factor for the probability of choosing candidates in the move adding a link. The fractions $N^2/2L$ and $2L/N^2$ would in this case disappear from equations (37) and (38). The two algorithms of course generate the same ensemble. However, the modified algorithm would have much worse acceptance rate for sparse networks since the chance that there is a link between two randomly chosen vertices on a sparse graph is very small. Most of the chosen pairs of vertices are not connected by a link and therefore the algorithm will do nothing since there is no link to remove.

This problem is absent for the algorithm which we described previously since in that case only existing links are chosen as candidates for removal. One can easily estimate that the probability of accepting a link removal (38) is not very small. Indeed, even for sparse graph the factor $e^{-\mu}2L/N^2$ in Eq. (38) is of order unity. In this case both $\exp(\mu)$ and $L$ for large $N$ grow proportionally to $N$ and their product balances the factor $N^2$ in the denominator. The algorithm has a finite acceptance rate which does not vanish when the system size grows.

As an exercise, let us consider an example of unweighted ($W_\alpha = 1$) graphs with $N = 3$. This ensemble consists of four graphs shown in table II. Their statistical weights can be easily found to be $1/3!$, $3e^{-\mu}/3!$, $3e^{-2\mu}/3!$, $e^{-3\mu}/3!$, so we expect that the frequency of occurrence in random sampling should be $1 : 3e^{-\mu} : 3e^{-2\mu} : e^{-3\mu}$. As we see in table II the results of Monte-Carlo simulations are in perfect agreement with this expectation.

| $\mu = 0$ | Theor. | Exp. | Theor. | Exp. | Theor. | Exp. | Theor. | Exp. |
|-----------|--------|------|--------|------|--------|------|--------|------|
| $\mu = 0$ | 0.125  | 0.375| 0.375  | 0.374| 0.125  | 0.126| 0.125  | 0.126|
| $\mu = 0.2$ | 0.166  | 0.408| 0.334  | 0.091| 0.166  | 0.166| 0.091  | 0.091|
| $\mu = 0.5$ | 0.241  | 0.439| 0.266  | 0.054| 0.241  | 0.241| 0.054  | 0.054|

TABLE II: Comparison of the probability distribution of graphs in a grand-canonical ensemble with $N = 3$ nodes: calculated theoretically and computed in a run of Monte-Carlo simulation in which $10^6$ graphs were generated.

One can easily apply this technique to any form of statistical weights. In particular we can consider the product weights (19). The probability of accepting a new configuration by adding or removing a link between $ij$ reads

$$min \left\{ \frac{1}{1 - \frac{N^2}{2(N + 1)}} \exp(-\mu) \frac{p(q_i + 1)p(q_j + 1)}{p(q_i)p(q_j)} \right\} \text{ for adding a link,}$$

$$min \left\{ \frac{1}{1 - \frac{2L}{N^2}} \exp(+\mu) \frac{p(q_i - 1)p(q_j - 1)}{p(q_i)p(q_j)} \right\} \text{ for deleting a link,}$$

where $L$ and $q_i, q_j$ refer to the current configuration.

### VIII. MONTE-CARLO GENERATOR OF MICRO-CANONICAL ENSEMBLE

Another frequently encountered ensemble is an ensemble of graphs which have a given node degree sequence $\{q_1, q_2, \ldots, q_N\}$. The partition function $Z$ has the form:

$$Z(N, \{q_i\}) = \sum_{\alpha \in q_i(N, L)} \left( \prod_{i=1}^{N} \delta [q_i(\alpha') - q_i] \right) 1/N! W(\alpha'),$$

where the product of delta functions allows one to include only those graphs which have a prescribed degree distribution $q_i$. As before the factor $1/N!$ is fixed in this ensemble and could in principle be skipped. The canonical partition function $Z(N, L)$ is related to the micro-canonical ones:

$$Z(N, L) = \sum_{q_1=0}^{\infty} \cdots \sum_{q_N=0}^{\infty} Z(N, \{q_i\}) \delta [q_1 + q_2 + \cdots + q_N - 2L].$$

To generate graphs from micro-canonical ensemble one has to have a Markov process preserving node degrees. The main idea is to combine simultaneous rewireings as shown in Fig. 4. We shall call this combination "X-move". At
FIG. 6: The idea of "X-move": two oriented links (dotted lines) $ij$ and $kl$ chosen in a random way are rewired, exchanging their endpoints. Then the opposite links (solid lines) are also rewired.

each step one picks up two random links: $ij$ and $kl$, and rewire them to $il$ and $kj$. This procedure is ergodic, i.e. it explores the whole configuration space. Such a transformation was discussed in [27] where it was used to randomize graphs with a given nodes’ degree sequence. In that case the functional weight was $W_\alpha = 1$ and rewirings were done with probability equal to one. In general case if one considers non-trivial $W_\alpha$, one has to accept the change with a corresponding Metropolis probability. In this way one can for example generate graphs whose statistical weights depend on the number of triangles. In a sense one can perform a weighted randomization of networks with the given node degree sequence. Introducing a weight into randomization may be very important in the construction of scoring functions in problems of motif searching. If one tries to determine relations between structural motifs and the functionality of network, it is very important to properly construct scoring function which may clearly account for the existence of a particular subgraph on a network and its function. Scoring functions are usually measured as a sort of distance between a network which displays a certain function and a random network which does not. An important problem in such studies is how to construct those networks which should serve as the background reference. The simplest idea is to use networks obtained by uniform randomization. This may however introduce some bias and may be misleading. Imagine for example that a motif which is responsible for a certain network function is built out of a couple of triangular loops and that triangular loops alone have no function. It is clear that one would like to control the abundance of triangular loops to distinguish between specific motifs and motifs which are more frequent by pure chance just because of higher abundance of triangles. Therefore it may be important to control the number of triangles in the randomized reference networks used in the scoring function. It was just an example, but in general case it might be useful to perform a weighted randomization taking into account some desired features of reference networks.

IX. GRAPH GENERATOR AND ADJACENCY MATRICES

All the elementary transformations: rewiring, adding or removing a link, and the X-move have a simple representation in terms of adjacency matrices. Rewiring relies on picking up at random an element $A_{ij} = 1$ of the adjacency matrix and flipping it with an element $A_{ik} = 0$ so that after the move $A_{ij} = 0$ and $A_{ik} = 1$. For undirected links adjacency matrices are symmetric and therefore at the same time one has to flip $A_{ji} = 1$ and $A_{ki} = 0$. To add a vertex one chooses at random $A_{ij}$ and if $A_{ij} = 0$ and $i \neq j$, one changes it into $A_{ij} = 1$ (and for $A_{ji}$ correspondingly). To remove a link one picks up a non-vanishing element $A_{ij} = 1$ and substitutes it with $A_{ij} = 0$. To perform X-move one picks up two non-vanishing elements of $A$ at random, say $A_{ij} = 1$ and $A_{kl} = 1$, and flips them simultaneously with $A_{il} = 0$ and $A_{kj} = 0$ to: $A_{ij} = 0$, $A_{kl} = 0$, $A_{il} = 1$ and $A_{kj} = 1$. Of course one also flips their four symmetric counterparts. In practice, when simulating sparse graphs one does not use the matrix representation since it would require $N^2$ storage capacity. For sparse matrices the number of non-vanishing matrix elements is proportional to $N$ and one can use a linear storage structure. It directly corresponds to the underlying graph structure. Using linear storage one can code graphs having of order $10^6$ nodes or even more on a PC.

X. DEGENERATED GRAPHS (PSEUDOGRAPHS)

In previous sections we described ensembles of simple graphs. Let us now discuss pseudographs that is graphs which may have multiple- and self-connections.

A degenerate undirected pseudograph can be represented by a symmetric adjacency matrix $A$ whose off diagonal entries $A_{ij}$ count the number of links between vertices $i$ and $j$, and the diagonal ones $A_{ii}$ count twice the number of self-connecting links attached to vertex $i$. For example, the graph depicted in Fig. 7 has the following adjacency
In the representation where each undirected link is represented as two opposite directed links all matrix elements including the diagonal ones count the number of directed links emerging from the vertex.

As before let us first consider labeled pseudographs. However, in order to have a unique representation of a graph one has to label links as well. We did not have to do this for simple graphs since in that case each link was uniquely determined by its endpoints. It is not anymore the case for degenerate graphs since there may be more than one link between two nodes. A pseudograph with \( N \) nodes and \( L \) links can be fully labeled by \( N \) node labels and \( 2L \) labels of directed links. Each fully labeled graph has thus the configuration space weight equal to \( 1/(N!(2L)!) \). Let us work out the consequences of this choice. Denote \( \alpha \) a graph, \( \alpha' \) a labeled graph of \( \alpha \) with labeled nodes only, and \( \alpha'' \) a fully labeled graph of \( \alpha \) with labeled nodes and labeled links. From here on labeled graph means a graph which has only labels on nodes while fully labeled graph a graph which has additionally labels on directed links.

The configuration space weight of \( \alpha \) can be calculated as a sum over all fully labeled graphs \( \alpha'' \) as follows:

\[
w_\alpha = \sum_{\alpha'' \in \text{flg}(\alpha)} \frac{1}{N!(2L)!} = \frac{1}{N!} \left( \prod_i \frac{1}{2^{A_{ii}/2} (A_{ii}/2)!} \right) \prod_{i>j} \frac{1}{A_{ij}!},
\]

(42)

where \( \text{flg}(\alpha) \) denotes the set of fully labeled graphs of graph \( \alpha \), \( \text{lg}(\alpha) \) the set of labeled graphs (labeled nodes only) of graph \( \alpha \). The expression \( A_{ii}/2 \) counts the number of self-connecting links attached to vertex \( i \), and \( A_{ij} \) is the multiplicity of links connecting \( i \) and \( j \). If there are no self-connections (\( A_{ii} = 0 \)) and no multiple connections (\( A_{ij} \leq 1 \)), the configuration space weight \( 42 \) reproduces the weight of simple graphs. One can easily understand the appearance of the combinatorial factors in general case. Suppose that we permute links’ labels of a fully labeled graph leaving nodes’ labels intact. Among all \( (2L)! \) permutations not all are distinct. If we have \( A_{ij} \) links between vertex \( i \) and \( j \) and we will permute their labels, then all \( A_{ij}! \) permutations will give the same labeled graph (if we simultaneously permute labels of the directed partners). Similarly if we have vertex with a self-connection and we exchange labels of the two directed links emerging from this vertex, the fully labeled graph will not change. Thus for each self-connection two permutations lead to the same fully labeled graph. To summarize, the number of distinct permutations of link labels is reduced from \( (2L)! \) by dividing out the factor 2 for each self-connection and \( k! \) for each \( k \)-link multiple connection which just gives Eq. (42). It turns out that these weights are identical to the combinatorial factors of Feynman diagrams which appear in perturbative series of a mini-field theory. One can thus interpret random pseudographs as Feynman diagrams and use perturbation theory to enumerate them.

Let us consider as an example a canonical ensemble of pseudographs with \( N = 3 \) and \( L = 3 \). There are 14 graphs in this ensemble. They are shown in Fig. 8. In table III we compare the theoretically calculated probability distribution of graphs:

\[
p_\alpha = \frac{w_\alpha}{\sum_\beta w_\beta},
\]

(43)

using the weights calculated by the formula \( 42 \) with the probability distribution obtained experimentally from the frequency histogram of graphs produced by the Monte-Carlo generator. Now the generator works exactly as before except that it does not reject moves leading to a self- or multiple-connections. The results are in perfect accordance.
As an example let us calculate the weight of graph M in Fig. 8. The weight of each labeled graph of graph M, according to the formula (42), is equal

$$w_M' = \frac{1}{3!} \cdot \frac{1}{2^3} \cdot \frac{1}{2!} = \frac{1}{96},$$

(44)

where the first factor comes from $1/N!$, the second from the three self-connections, and the third from the fact that the two self-connections are attached to the same vertex and thus can be permuted without changing graph’s connectivity. There are six distinct labeled graphs $M'$ of graph M and thus

$$w_M = \sum_{M'} \frac{1}{96} = \frac{6}{96} = \frac{1}{16}.$$

(45)

One should note that the number of distinct labeled graphs varies from graph to graph. For example, for graph L there is only one labeled graph. In this case $w_L = 1/3! \cdot 1/2^3 = 1/48$ and $w_L = 1/48$. The calculation can be easily repeated for each graph in Fig. 8 yielding the weights $w_\alpha$ listed in Table III.

As follows from Eq. (42), the partition function for the canonical ensemble of pseudographs can be written in three different ways:

$$Z(N, L) = \sum_{\alpha' \in lg(N, L)} \frac{1}{N!(2L)!} = \sum_{\alpha' \in lg(N, L)} \frac{1}{N!} \left( \prod_i \frac{1}{2A_{ii}/2!} \right) \prod_{i>j} \frac{1}{A_{ij}!} = \sum_{\alpha \in g(N, L)} w_\alpha.$$

(46)

The first sum runs over fully labeled graphs and has the simplest form since all fully labeled graphs have the same weight. The weight of labeled graphs in the second sum varies. We note that labeled graphs are isomorphic with adjacency matrices that is each labeled graph is uniquely represented by a generalized adjacency matrix [37] like Eq. (41). The sum over $\alpha' \in lg(N, L)$ can be thus interpreted as a sum over all generalized adjacency $N \times N$ symmetric matrices $A$ such that $\sum_{ij} A_{ij} = 2L$. We see that not all adjacency matrices have the same statistical weight unlike for simple graphs since the weights depend on the number of self- and multiple-connections.

A weighted ensemble of pseudographs is constructed as before by introducing an additional functional weight $W(\alpha)$
under the sum defining the partition function (46):

\[
Z(N, L) = \sum_{\alpha'' \in g(N, L)} \frac{1}{N!(2L)!} W(\alpha'') = \sum_{\alpha \in g(N, L)} w_\alpha W(\alpha).
\]

As before the functional weight \( W(\alpha'') \) does not depend on graph’s labeling but only on graph’s topology. In other words if \( \alpha''_1 \) and \( \alpha''_2 \) are two different fully labeled graphs of graph \( \alpha \) then \( W(\alpha''_1) = W(\alpha''_2) \equiv W(\alpha) \).

We can now consider various weights: for example a product weight as in Eq. (19) to mimic graphs with uncorrelated node degrees. But even in this case the total weight does not factorize since the configuration space weight \( w(\alpha) \) written as a function of node degrees \( w(q_1, q_2, \ldots, q_N) \) does not factorize. Due to the absence of the structural constraints the approximation given by equations (20) and (21) has now much weaker finite size corrections.

A grand-canonical ensemble for pseudographs with arbitrary product weights (19) has the following partition function:

\[
Z(N, \mu) = \sum_{L} \exp(-\mu L) \sum_{\alpha \in g(N, L)} w_\alpha \prod_{i=1}^{N} p(q_i(\alpha)).
\]

This means that all pseudographs with fixed nodes’ degrees \( \{q_i\} \) have the same functional weight \( \sim p(q_1) \cdots p(q_N) \), which seems to be similar to that generated by the Molloy-Reed construction of pseudographs [31]. Let us comment on this. In the Molloy-Reed construction one generates a sequence of non-negative integers \( \{q_1, q_2, \ldots, q_N\} \) as independent identically distributed numbers with the distribution \( p(q) \). One interprets \( q_i \)’s as node degrees. The only requirement is that the sum \( q_1 + q_2 + \cdots + q_N = 2L \) is even. In the first step of the construction each integer \( q_i \) is represented as a hub built out of a vertex and \( q_i \) outgoing branches which can be viewed as directed links emerging from this vertex. In the second step the directed links are paired randomly in couples of links in opposite direction to form undirected links connecting vertices. This procedure generates the same subset of pseudographs as the partition function \( Z(N, \mu) \) [18]. However, statistical weights are different.

To see this, let us consider a subset of Molloy-Reed graphs obtained for a given set \( \{q_i\} \). There are \( N \) labeled vertices and \( 2L = \sum q_i \) labeled directed links. All permutations of labels of links and nodes are equiprobable exactly as it was before for fully labeled pseudographs [12]. If one calculates corresponding symmetry factors for node-labeled graphs the same combinatorial factors arise as in Eq. (22): if one pairs two directed links \( a \) and \( b \) which belong to the same vertex one obtains a self-connecting link. The pair \( ab \) is identical as \( ba \) since both the links begin and end at the same vertex. This reduces the number of distinct permutations by factor of \( 2 \) as in Eq. (22). Similarly for \( k \) pairs of directed links between two vertices one can exchange the order of pairing in \( k! \) ways each time obtaining the same multiple connection, so the corresponding factor is \( 1/k! \) again as in Eq. (22). The conditional probability of choosing a particular graph \( \alpha \) under the condition that in the first step of the construction the set of \( \{q_1, q_2, \ldots, q_N\} \) has been selected, is

\[
w_{M-R}(\{q_i\}|\alpha) = \frac{w_\alpha}{\sum_{\beta \in g(q_1, \ldots, q_N)} w_\beta},
\]

where the sum is done over all (unlabeled) pseudographs \( \beta \) from the micro-canonical set of fixed degrees \( \{q_1, \ldots, q_N\} \).

The total probability is thus

\[
w_{M-R}(\alpha) = P(\{q_i\}) w_{M-R}(\{q_i\}|\alpha),
\]

where \( P(\{q_i\}) \) is the probability that in the first step of the construction the set \( \{q_1, \ldots, q_N\} \) is selected. This probability is proportional to the product of \( p(q_i) \)’s multiplied by the number of permutations of \( \{q_1, \ldots, q_N\} \) which give the same set. We denote this number by \( \text{Perm}(q_1, \ldots, q_N) \). The order of \( q_i \)’s does not matter since we consider unlabeled graphs. For example, the following permutations (sequences): \( (q_1, q_2, q_3) = (3, 3, 2), (3, 2, 3) \) and \( (2, 3, 3) \) give the same set \( \{3, 3, 2\} \), so in this case we have \( \text{Perm}(3, 3, 2) = 3 \). In general, the number is given by

\[
\text{Perm}(q_1, \ldots, q_N) = \frac{N!}{n_0!n_1! \cdots},
\]

where \( n_0, n_1, \ldots \) are degree’s multiplicities: \( n_q = \sum_i \delta[q_i - q] \). Thus

\[
P(\{q_i\}) \propto \left( \prod_{i=1}^{N} p(q_i(\alpha)) \right) \text{Perm}(\{q_i\}).
\]
Collecting all the factors together and normalizing to have the probabilistic interpretation we obtain the following expression for the total weight (probability) for Molloy-Reed’s pseudographs:

\[ w_{M-R}(\alpha) = \left( \prod_{i=1}^{N} p(q_i(\alpha)) \right) \frac{\text{Perm}(q_1(\alpha), \ldots, q_N(\alpha))}{\sum_{k_1, \ldots, k_N} \text{Perm}(k_1, \ldots, k_N) \sum_{\beta \in g(q_1, \ldots, q_N)} w_\beta} \]  

(53)

The first factor comes from picking \( N \) numbers \( q_i \) at random, the second counts permutations and the third includes the weight generated by pairing directed links. As we see, despite many similarities the Molloy-Reed ensemble and the grand-canonical lead to different weights. As an example, in Fig. 9 we show an ensemble of 10 pseudographs with \( N = 3 \) generated by Molloy-Reed algorithm for \( p(q) = 1/3 \) for \( q = 0, 1, 2 \) and zero elsewhere. We compare statistical weights of the generated graphs with the corresponding ones in the grand-canonical ensemble. As we can see in table IV the weights are different in the two ensembles.

**Summary**

We have discussed a statistical approach to homogeneous random graphs. This framework is a natural extension of the Erdős-Rényi theory to the case of weighted graphs: one considers the same set of graphs but with modified statistical weights. The statistical weights of homogeneous graphs depend only on graphs’ topology. In other words, if one assigns some labels to its nodes, they will have no physical meaning similarly as the numbers of indistinguishable particles in quantum mechanics. One can permute them and the graph and its statistical weight will stay intact. The only information which matters is the number (entropy) of distinct permutations of nodes’ labels. All permutations of node’s labels are equivalent, unlike for growing networks where those permutations have to preserve the causal order corresponding to the order of node’s attachment to the graph. The statistical weight of a homogeneous graph is proportional to the number of all labeled graphs of this graph while of a growing network to the number of causally labeled graphs. This leads to a difference between homogeneous and growing networks. For example, a typical homogeneous graph has a larger diameter than the corresponding growing network with the same node.

### TABLE IV: Weights calculated for the Molloy-Reed construction and for the corresponding grand-canonical ensemble with \( N = 3 \). For each sequence \( q_1, q_2, q_3 \) we give the combinatorial number \( \text{Perm}(q_1, q_2, q_3) \) of permutations leading to the same graph. Altogether, there are 14 different sequences of length three, with \( q_i = 0, 1 \) or 2 as can be seen in the third column of the table.

| \( L \) \{ \( q_i \) \} | \( \text{Perm}(q_1, q_2, q_3) \) | \( \text{Graphs} \) | \( w_\alpha \) weights | \( w_{M-R} \) weights | G-C weights from Eq. 48 |
|---|---|---|---|---|---|
| 3 2,2,2 | 1 | A1,A2,A3 | \( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} = \frac{1}{8} (8 : 6 : 1) \) | \( \frac{1}{16} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) | \( e^{-3\mu} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) |
| 2 2,2,0 | 3 | B1,B2 | \( \frac{1}{2} : \frac{1}{1} = \frac{1}{2} (1 : 2) \) | \( \frac{1}{15} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) | \( e^{-2\mu} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) |
| 2,1,1 | 3 | C1,C2 | \( \frac{1}{3} : \frac{1}{2} = \frac{1}{2} (2 : 1) \) | \( \frac{1}{15} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) | \( e^{-2\mu} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) |
| 1 2,0,0 | 3 | D | \( \frac{1}{1} : \frac{1}{1} = \frac{1}{1} (1 : 1) \) | \( \frac{1}{15} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) | \( e^{-\mu} \frac{1}{1} \) |
| 1,1,0 | 3 | E | \( \frac{1}{2} : \frac{1}{1} = \frac{1}{1} (1 : 1) \) | \( \frac{1}{15} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) | \( e^{-\mu} \frac{1}{1} \) |
| 0 0,0,0 | 1 | F | \( \frac{1}{1} : \frac{1}{1} = \frac{1}{1} (1 : 1) \) | \( \frac{1}{15} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) | \( \frac{1}{15} \left( \frac{1}{2} : \frac{1}{2} : \frac{1}{2} \right) \) |
degree distribution \[13\]. Generally, geometrical properties of homogeneous graphs are different from those of growing networks for which correlations between the time of node’s attachment and its degree induce node-node correlations of a specific type \[12, 13\]. Such correlations are absent for homogeneous graphs.

Various functional properties of homogeneous networks can be modeled by an appropriate choice of functional weight. One can easily produce networks with an assertive mixing, higher clustering or any desired property which can reflect any real-data observation.

Homogeneous networks can be simulated numerically. We have also described a Monte-Carlo algorithm to generate canonical, grand-canonical and micro-canonical ensembles which performs a sort of weighted random walk (Markov chain) in the configuration space with a desired stationary distribution. We advocated the importance of the possibility of generating random networks with desired statistical properties for advanced motif searching \[28, 29, 30\].

Many real networks have resulted from hybrid processes of growth mixed with some thermalization. The framework discussed in this paper can flexibly extrapolate between the two regimes. It allows one to directly investigate the relation between structural and functional properties of complex networks.

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\[32\] For simple graphs it is immaterial to label links since each link is uniquely determined by its end points.
\[33\] At first glance one can think that there are six ways because one can put labels in six different ways on a drawing of the triangle. After a while one can see that they are all identical since they can be transformed one into another by a transformation which does not change connectivity. For example, if it is a drawing of equilateral triangle one can change labels 123 into 231 by rotating it by 120°.
\[34\] One should however remember that this constant is an irrelevant proportionality factor as long as the number of nodes is fixed.
\[35\] One can show that all eigenvalues of a Markov transition matrix lie inside or on the unit circle \(|\lambda| \leq 1\).
Even if a rewiring is rejected we count it in since it corresponds to the transition \( P(\alpha \to \alpha) \) from graph to the same graph. The elements \( A_{ij} \) are indexed by nodes’ labels, but the information about links’ labels is lost in the adjacency matrix representation.