

An algorithm for counting circuits: Application to real-world and random graphs

E. MARINARI¹, R. MONASSON² and G. SEMERJIAN³

¹ *Dipartimento di Fisica and INFN, Università di Roma La Sapienza
P. A. Moro 2, 00185 Roma, Italy*

² *CNRS-Laboratoire de Physique Théorique de l'ENS - 24 rue Lhomond
75005 Paris, France*

³ *Dipartimento di Fisica and SMC-INFN, Università di Roma La Sapienza
P. A. Moro 2, 00185 Roma, Italy*

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Abstract. – We introduce an algorithm which estimates the number of circuits in a graph as a function of their length. This approach provides analytical results for the typical entropy of circuits in sparse random graphs. When applied to real-world networks, it allows to estimate exponentially large numbers of circuits in polynomial time. We illustrate the method by studying a graph of the Internet structure.

Introduction. – An increasing amount of data has been collected on the topology of real-world networks appearing in many different contexts, the Internet being only one of many examples [1]. A natural line of research in this field consists in identifying characteristic features of the networks, to compare them with theoretical models and potentially disprove the latter. The simplest of these properties is the distribution of vertex degrees, which has been repeatedly argued to exhibit power law tails. Quite generally, it is computationally easy to measure the “local” (involving a vertex and a finite number of neighbors) properties of a given network; for instance, loops with less than 5 edges in the Internet graph have been studied in [2]. However, it might well be that the most distinctive features of real-world networks are “global” (*i.e.* that they depend on an extensive portion of the graph): their measure becomes then a very challenging numerical problem.

Among these global properties, we shall consider in the present work the number of long circuits in a graph, *i.e.* of circuits visiting a finite fraction of the vertices [3]. These circuits are roughly exponentially numerous in the size of the graph: because of that the use of exact algorithms [4], whose complexity is linear in the number of cycles to be enumerated, is possible for small sizes only. Another trace of this difficulty lies in the NP-completeness of the decision problem of knowing if a graph is Hamiltonian (*i.e.* if it contains a loop visiting all vertices) [5]. To overcome this difficulty it is reasonable to look for approximate algorithms with running times scaling polynomially with the network size. A formal result in this direction is the existence of a probabilistic algorithm for the approximate counting of Hamiltonian cycles in

graphs with large minimal connectivity [6]. Very recently a sampling method based on a Monte Carlo Markov Chain has been proposed [7].

In this letter we introduce a counting algorithm, relying on a statistical mechanics approach expanding on the results of [8] (see also [9]), the details of which shall be exposed in a longer publication [10]. The algorithm is first applied to a real-world network, then to random graphs. In the latter context the number of circuits of a given length is a random variable, whose properties have been thoroughly studied by Garmo [11] in the regular case (all vertices have the same degree, see also [12] for a review). For the Erdős-Rényi ensemble (in which vertex degrees are Poisson distributed), most results have been obtained in the vicinity of the percolation transition, or on the contrary for very large average degrees [13]. The calculation of the expected number of circuits in ensembles with arbitrary degree distributions has been recently performed by Bianconi and Marsili [14]. However, these expectations turn out to be dominated by atypical (exponentially rare) graphs with exponentially more circuits than the typical ones.

Definitions and algorithm. – Let $G = (V, E)$ be a graph, where V and E are the sets of vertices and edges, respectively. The size of G is the number of vertices, $N = |V|$. A circuit $\mathcal{C} = (V_{\mathcal{C}}, E_{\mathcal{C}})$ is a closed path on the graph visiting each vertex at most once. The length L of the circuit is the number of visited vertices or edges, $L = |V_{\mathcal{C}}| = |E_{\mathcal{C}}|$. A circuit visiting all vertices ($L = N$) is called Hamiltonian. Our scope is to count the number of distinct circuits of a given graph G , $\mathcal{N}_L(G)$, as a function of their length L ; more precisely, we define below a procedure estimating the entropy $\sigma(\ell) = (\ln \mathcal{N}_L)/N$ of circuits of length $N\ell$. The reduced length ℓ is an intensive parameter in $[0, 1]$. For $i \in V$, we call ∂i the set of neighbors of the vertex i , and use the symbol \setminus to subtract an element of a set: if j is a neighbor of i , $\partial i \setminus j$ will be the set of all neighbors of i distinct from j . We denote by $i \rightarrow j, j \rightarrow i$ the two oriented edges that can be built from $(ij) \in E$: see fig. 1 for an illustration of these definitions.

The basic idea of our approach is to introduce a probability law $p(\mathcal{C}; G, u) = u^{|\mathcal{C}|}/Z(G, u)$ over the set of circuits of G . Hence the normalization factor $Z(G, u) = \sum_{\mathcal{C}} u^{|\mathcal{C}|}$ is equal to the generating function of the number of circuits, $\sum_L \mathcal{N}_L(G)u^L$. In the limit of large graphs and circuit lengths, the saddle point method leads to the relation $\frac{1}{N} \ln Z(G, u) = \max_{\ell} [\sigma(\ell) + \ell \ln u]$. This relation can be inverted with standard Legendre transformations, and the entropy σ can be expressed in terms of the partition function Z . An estimate of Z can then be obtained by using the Bethe approximation of the corresponding statistical mechanics model, or by means of Monte Carlo simulation [7]. Following the former road, and using the well-known correspondence between minimization of the Bethe free energy and iterations of the Belief Propagation equations [15], one is lead to the following algorithm (see [10] for details):

Circuit Counting Algorithm

Input: a graph $G = (V, E)$, u a real positive number.

Operation: iterate the set of $2|E|$ recursive equations

$$y_{i \rightarrow j}^{(T+1)} = \frac{u \sum_{m \in \partial i \setminus j} y_{m \rightarrow i}^{(T)}}{1 + \frac{1}{2}u^2 \sum_{\substack{m, n \in \partial i \setminus j \\ m \neq n}} y_{m \rightarrow i}^{(T)} y_{n \rightarrow i}^{(T)}}, \quad (1)$$

from a randomly chosen initial condition $y_{i \rightarrow j}^{(0)} > 0$ until it converges (within some *a priori* accuracy) to a fixed point $y_{i \rightarrow j}^*(G, u)$.

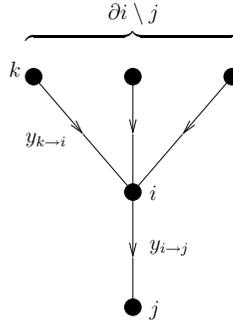


Fig. 1 – A vertex i , and its neighbors j and $k \in \partial i \setminus j$. Each oriented edge carries a message y involved in eq. (1).

Output: estimate of the entropy $\sigma(\ell)$ of circuits of length $N \ell$ with

$$\ell = \frac{1}{N} \sum_{(ij) \in E} p_{(ij)}, \quad p_{(ij)} = \frac{u y_{i \rightarrow j}^* y_{j \rightarrow i}^*}{1 + u y_{i \rightarrow j}^* y_{j \rightarrow i}^*}, \quad (2)$$

$$\sigma(\ell) = \frac{1}{N} \sum_{i \in V} \ln \left(1 + \frac{1}{2} u^2 \sum_{\substack{m, n \in \partial i \\ m \neq n}} y_{m \rightarrow i}^* y_{n \rightarrow i}^* \right) - \frac{1}{N} \sum_{(ij) \in E} \ln (1 + u y_{i \rightarrow j}^* y_{j \rightarrow i}^*) - \ell \ln u.$$

The procedure has to be repeated with different values of u to reconstruct a parametric plot of $\sigma(\ell)$ for $\ell \in [0; \ell_{\max}]$. For small values of u , the iteration equations converge to the trivial solution, $y^* = 0$ for all edges. The minimal value of u yielding a non-trivial solution, u_0 , is related to the slope of the entropy at the origin, $d\sigma/d\ell|_0 = -\ln u_0$.

The algorithm runs in time growing polynomially with the graph size and logarithmically with the required accuracy on the fixed-point solution. For generic graphs, one cannot warrant neither the convergence of the iteration, nor the validity of the Bethe approximation (see [16] for the computation of corrections). This approximation is, however, expected to be correct for large random graphs, and should be reasonable for most real-world networks.

Besides the global information $\sigma(\ell)$, the algorithm gives a local description of the circuits of the graph, through the quantities y^* , called *messages* hereafter. These have indeed the following interpretation: for $(ij) \in E$, $p_{(ij)}$ defined in eq. (2) is the probability that the edge is present in a circuit \mathcal{C} drawn from the distribution $p(\mathcal{C}; G, u)$, *i.e.* the fraction of the circuits of length ℓ which go through (ij) .

Note that in eq. (1) we used the convention that sums on empty sets are null. In particular, $y_{i \rightarrow j} = 0$ if i is the only neighbor of j , in other words if i is a leaf of the graph. Moreover, if all incoming messages on a edge are vanishing, the outgoing message is also null. This simple remark implies that edges (ij) with at least one of their fixed-point messages $y_{i \rightarrow j}^*, y_{j \rightarrow i}^*$ vanishing are exactly the ones which would be erased in the leaf removal procedure to compute the 2-core (maximal subgraph in which all vertices have degree at least 2) of the graph [17]. This property could be expected: by definition, no circuit can be drawn outside of the 2-core.

Application to real-world graphs: approximate counting. – As an illustrative example, we present in fig. 2 the output of the algorithm when applied to the graph of the Internet structure at the Autonomous Level System, using preliminary data from the DIMES measurement project [18]. The original graph contained $N = 14291$ vertices and $M = 33666$ edges.

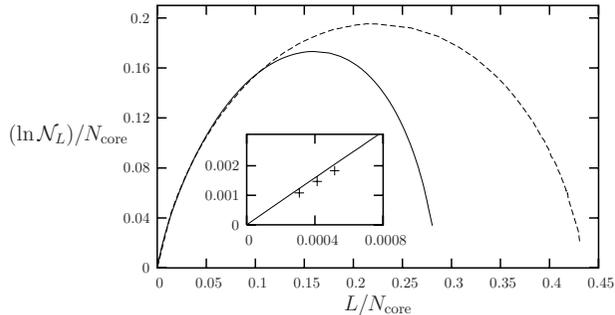


Fig. 2 – Solid line: the number of circuits in a graph of the Internet. Inset: magnification of the small-length results, the symbols have been obtained by exhaustive enumeration of the circuits of length $L = 3, 4, 5$. Dashed line: typical entropy in the random graph ensemble of same connectivity distribution.

For simplicity, we plot the results in units of its 2-core size, $N_{\text{core}} = 9694$ (the 2-core contains $M_{\text{core}} = 29069$ edges). Two features of this entropy curve can be underlined. According to our algorithm, the most numerous circuits contain 1555 edges, and there are around 10^{729} (certainly out of reach of any direct enumeration) of such circuits; the longest ones contain $L_{\text{max}} \approx 2710$ edges. The agreement between exact enumerations for short circuits of length $L = 3, 4, 5$ (enumerating longer ones becomes excessively costly) and the results of the algorithm is quantitatively decent (see inset of fig. 2). A rough analysis of the local information provided by the algorithm shows that high degree vertices belong generally to a higher fraction of circuits than poorly connected ones; there are however strong fluctuations around this general trend.

Application to random graphs: analytical results. – Consider now random-graph ensembles with fixed degree distribution, and call q_k the fraction of vertices having degree k . We assume that q_k decays fast enough for large connectivities, so that all its moments are well defined. Let us introduce the average degree c , and the probability that the end-vertex of a randomly chosen edge has degree $k + 1$, $\tilde{q}_k = (k + 1)q_{k+1}/c$. The typical (quenched) entropy density is defined by $\sigma_q(\ell) = \ln \overline{\mathcal{N}_{\ell N}(G)}/N$, where the over-line denotes an average over the random-graph ensemble. In contrast the computation of [14] yields the annealed entropy $\sigma_a(\ell) = \ln \mathcal{N}_{\ell N}(G)/N$.

Running the algorithm defined above on a graph of the ensemble leads to a random (with respect to the choice of the graph) set of messages y^* . The assumptions of the so-called cavity method at the replica-symmetric level [19] lead to a self-consistent equation for the distribution P of the messages y found on a randomly chosen directed edge:

$$\begin{aligned}
 P(y; u) = & \tilde{q}_0 \delta(y) + \sum_{k=1}^{\infty} \tilde{q}_k \int_0^{\infty} \prod_{m=1}^k dy_m P(y_m; u) \times \\
 & \times \delta \left(y - g \left(\sum_{m=1}^k y_m, \sum_{m=1}^k y_m^2, u \right) \right), \quad (3)
 \end{aligned}$$

where $g(a, b, u) = ua/(1 + u^2(a^2 - b)/2)$ (see eq. (1)). From the solution of this distributional equation, easily found numerically by means of a population dynamics algorithm [20], one can use eq. (2) to compute the typical entropy of the graphs of the ensemble, $\sigma_q(\ell)$, parametrized by u . We present in fig. 3 the results of this approach on Poissonian graphs (*i.e.* $q_k = e^{-c}c^k/k!$)

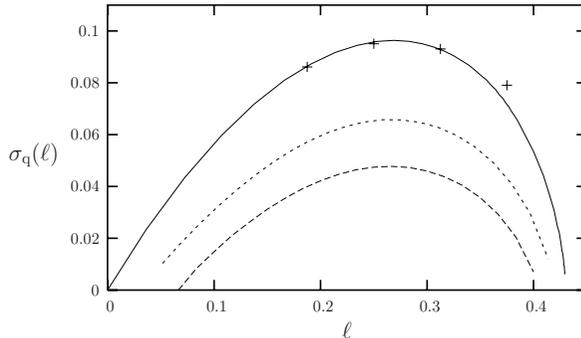


Fig. 3 – Typical entropy for Poissonian graphs with $c = 2$, cavity computation (solid line) and exhaustive enumeration determination of the median number of cycles in samples of 200000 graphs of size $N = 60$ (long-dashed line) and $N = 116$ (short-dashed line). Symbols obtained by an extrapolation of the numerical results for several values of N to the limit $N \rightarrow \infty$.

with mean degree $c = 2$, along with a confirmation by exhaustive enumeration on finite-size samples.

An analytic resolution of eq. (3) is possible only for the very particular case of random regular graph for which all q_k but one vanish. We find that P reduces to a single Dirac distribution in $y^*(c)$ solution of $y^* = g((c-1)y^*, (c-1)(y^*)^2, u)$. In that case the fluctuations of \mathcal{N}_L are sufficiently small for the annealed and quenched averages to coincide and the result obtained rigorously in [11] is found back [8].

Some analytical predictions can be made when the random graphs are not purely regular, even if P is not known explicitly. First of all, the fraction ζ of strictly vanishing messages is found to be the smallest root in $[0; 1]$ of $\zeta = \sum_{k \geq 0} \tilde{q}_k \zeta^k$. Following the above interpretation of the null messages, the fraction of edges that belong to the 2-core is $(1 - \zeta)^2$. Moreover, its connectivity distribution can also be expressed from ζ and \tilde{q}_k , and these predictions checked from the solution of the differential equations describing the leaf removal algorithm [10, 17].

One can also set up a systematic expansion of σ_q around $\ell = 0$. To state the results in a compact way, let us define the factorial moments of \tilde{q}_k as $\tilde{\mu}_n = \sum_{k \geq n} \tilde{q}_k k(k-1) \dots (k-n+1)$.

The coefficients of the second-order expansion of the entropy read

$$\left. \frac{d\sigma_q}{d\ell} \right|_0 = \ln \tilde{\mu}_1, \quad \left. \frac{d^2\sigma_q}{d\ell^2} \right|_0 = -\frac{1}{c} \left(\frac{\tilde{\mu}_3}{\tilde{\mu}_1^2} + \frac{2\tilde{\mu}_2^2}{\tilde{\mu}_1^3(\tilde{\mu}_1 - 1)} \right). \quad (4)$$

Comparing this expansion with the annealed computation of [14], one finds that the first derivatives are equal in both computations, and match the known results for circuits of finite size. However, the second derivatives turn out to be different,

$$\left. \frac{d^2\sigma_a}{d\ell^2} \right|_0 - \left. \frac{d^2\sigma_q}{d\ell^2} \right|_0 = \frac{2}{c\tilde{\mu}_1^3(\tilde{\mu}_1 - 1)} (\tilde{\mu}_2 - \tilde{\mu}_1(\tilde{\mu}_1 - 1))^2. \quad (5)$$

It is straightforward to show from eq. (5) that the expansion of the annealed and quenched entropies coincide only if the distribution \tilde{q}_k is supported by a single integer, in other words in the random regular graph case.

Another limit that can be investigated analytically is the one of maximal length circuits ℓ_{\max} , reached here when u gets large. We need to distinguish two cases: if the connectivity distribution is supported on the integers larger than 3, the cavity computation predicts

$\ell_{\max} = 1$, and the graphs in such ensembles are typically Hamiltonian. Interestingly, this was conjectured by Wormald in [12]. Even if the present statistical-mechanics approach does not provide a rigorous proof of the conjecture, it allows to make it quantitative (with the prediction of the typical entropy of such Hamiltonian circuits, $\sigma_q(1)$). Moreover, it gives a hint at why usual probabilistic methods are not powerful enough to prove the conjecture (the quenched entropy is strictly smaller than the annealed one in general). Note that this property concerning Hamiltonian circuits crucially relies on the fast decay of the degree distribution: it was shown in [14] that it can be invalidated when q_k has power law tails.

As soon as the connectivity distribution of the 2-core contains a finite fraction of sites of degree 2, it cannot be Hamiltonian. Consider indeed a vertex of degree k , surrounded by k' neighbors of degree 2, with $k \geq k' \geq 3$: it is obvious that no circuit can visit more than two of these k' sites. As the number of such forbidden vertices is extensive, one has $L_{\max}/N_{\text{core}} < 1$. The quantity ℓ_{\max} can be computed by taking analytically the appropriate limit in eq. (3) on P , resulting in a simpler distributional equation which can be solved analytically in the limit of infinitesimal fraction of degree-2 sites [10].

Discussion and conclusion. – We mentioned in the introduction the possibility of using global properties of graphs to test the relevance of random-graph ensembles for the description of real-world networks. Following this idea, we compared the circuit entropy of the DIMES Internet graph with the quenched result for the ensemble with the same connectivity distribution (dashed line in fig. 2). They turn out to be rather different, suggesting that random-graph ensembles defined only through their connectivity distribution are not a very precise description of real-world networks. It would thus be interesting to extend our analytical study to different ensembles of graphs, for instance introducing correlations between the degrees of neighboring vertices [21], or considering growing models of networks [22].

Concerning the application of the algorithm to individual graphs, two questions should be further investigated: can one give general conditions [23, 24] on the graphs which ensure the convergence of the BP equations? Can they be sharpened to show that the output of the algorithm is a rigorous lower bound on the true number of circuits? Tests on various types of graphs show that the iteration procedure is generally very robust against the initial condition on the y 's, and converges to a unique fixed point. Small counter-examples on which the BP equations do not converge can however be easily tailored.

Large deviations of \mathcal{N}_L around its typical value $e^{N\sigma_q(\ell)}$ could also be an interesting object of study, using for instance the modified cavity method of [25]. One may, in particular, seek the exponentially small probability that a randomly drawn graph is not Hamiltonian for ensembles whose typical instances are.

Finally, we hope that our algorithm will be useful for analyzing graphs data available in various contexts besides the Internet, *e.g.*, regulatory and more generally biological interaction networks. The huge size of these data sets make the use of exact analysis procedures impossible, not-to-say unnecessary when data are plagued by false positives and/or negatives as is often the case in biological experiments, *e.g.*, DNA chips. Approximate and fast algorithms may then reveal adequate.

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