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Temperature in complex networks

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Various statistical-mechanics approaches to complex networks have been proposed to describe expected topological properties in terms of ensemble averages. Here we extend this formalism by introducing the fundamental concept of graph temperature, controlling the degree of topological optimization of a network. We recover the temperature-dependent version of various important models as particular cases of our approach, and show examples where, remarkably, the onset of a percolation transition, a scale-free degree distribution, correlations and clustering can be understood as natural properties of an optimized (low-temperature) topology. We then apply our formalism to real weighted networks and we compute their temperature, finding that various techniques used to extract information from complex networks are again particular cases of our approach.

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Complex networks have recently attracted much interest from the community of physicists, due to the possibility of applying various techniques generally inspired by statistical mechanics in order to highlight universal properties [1, 2]. Among the several approaches that have been explored, an interesting one (originally proposed by sociologists and termed *exponential random graphs* [3]) has been recently explored within an explicit statistical-mechanics framework [4, 5, 6, 7, 8, 9]. This powerful formalism allows one to treat in a unified fashion a large class of models, including random graphs [1, 2], the configuration model [10], hidden-variable models [7, 8] and generalizations of them [6, 9]. If we restrict ourselves to unweighted networks with a fixed number of vertices N and with no self-loops or multiple edges, each link is regarded as a "particle" that can be placed between any two vertices, subject to the constraint that the "occupation number" of each pair of vertices i, j can only be $a_{ij} = 0, 1$ as in the familiar Fermi statistics. Clearly, a_{ij} coincides with the entries of the $N \times N$ adjacency matrix A characterizing the topology completely. Each allowed adjacency matrix A corresponds to a possible configuration, and the set of possible configurations (each with its statistical weight P_A) defines the statistical ensemble of graphs.

The above framework allows one to develop the statistical mechanics of networks by exploiting a range of tools which are well known in physics [6]. However, this thermodynamical analogy has not been fully explored yet. In particular, the concept of *temperature*, which is of key importance in the study of statistical ensembles, has received little or no attention until now in the literature on complex networks. Our aim in the present paper is to fully develop the thermodynamical formalism in order to include the temperature of a graph explicitly. As we report below for several particular cases including theoretical models and empirical data, we find intriguing results showing that the temperature allows for an additional understanding of complex networks. In particular we find that many well-known topological properties such as the presence of a giant component, a scale-free degree distribution, correlations and clustering can be easily understood in terms of the low-temperature behaviour of real networks. Our results can also be exploited to compute the temperature of real networks directly.

The reason for introducing the temperature of a network is because in our view the statistical formalism is incomplete without it. In all the approaches to exponential random graphs, the probability P_A depends on the *energy* E_A of the graph A, representing the *cost* of realising A. Now, this concept of cost is unclear without the assessment of its relative role with respect to the available *resources* that can be exploited to form the network. The relative importance of cost and available resources is usually controlled in statistical physics by the temperature. In the zero-temperature regime the system is forced to severe optimization, so that only the least costly configuration can be formed and the units of the system occupy the states with lowest energy (this is the *optimized* case). In the opposite, infinite-temperature extreme the system does not distinguish between cheap and expensive states, so that all configurations occur with the same probability. The formalism that we develop here is particularly suitable to model networks subject to such economic/engineering constraints. We shall complement the standard results obtained in the literature for the generic finite-temperature case (which is recovered when $T = 1$) with the interesting ones corresponding to zero and infinite temperature, which are not accessible to current finite-temperature models. A range of interesting results can be obtained by even the simplest models when T is allowed to vary, in particular when $T = 0$. Our approach works equally well for directed as well as undirected graphs, but for the sake of simplicity we write all

the expressions for the undirected case only. The generalization to directed graphs is straightforward.

The most general statistical ensemble for an equilibrium undirected network is a *grandcanonical* one [9] with $2^{N(N-1)/2}$ graphs having a fixed number of vertices N and a varying number of links $L_A = \sum_{ij} a_{ij}$, controlled by the chemical potential μ. If the temperature is explicitly introduced, the probability of graph A is

$$P_A = \frac{1}{\mathcal{Z}} \exp\left[\frac{\mu L_A - E_A}{T}\right] \qquad (1)$$

where $\mathcal{Z} \equiv \sum_A \exp(\mu L_A - E_A)/T$ is the *grand partition function* of the ensemble. Note that when $T \to \infty$ we have $P_A = 2^{-N(N-1)/2}$ for all graphs, while when $T \to 0$ we have $P_A = 1$ for the graph with the maximum value of $\mu L_A - E_A$ (or $P_A = M^{-1}$ if there are M degenerate such graphs), and $P_A = 0$ for all other graphs. The energy E_A can be in general an arbitrarily complicated function of the adjacency matrix A, but throughout the present paper we consider the instructive case, explored in most models, where it can be written as a sum over the individual link energies ϵ_{ij} [6, 9]: $E_A \equiv \sum_{ij} a_{ij}\epsilon_{ij}$. This allows us to write

$$\mathcal{Z} = \sum_{\{A\}} \prod_{ij} e^{(\mu-\epsilon_{ij})a_{ij}/T} = \prod_{ij} \left[1 + e^{(\mu-\epsilon_{ij})/T}\right] \qquad (2)$$

and $P_A = \prod_{ij} p_{ij}^{a_{ij}} (1-p_{ij})^{1-a_{ij}}$, where

$$p_{ij}(T) = \frac{1}{e^{(\epsilon_{ij}-\mu)/T} + 1} \qquad (3)$$

is the probability that a link between i and j exists, which has the usual form of Fermi statistics (alternative derivations of the above form for p_{ij} are given in refs.[6, 9] for $T = 1$). Therefore the additivity of E_A implies that each link is drawn with probability p_{ij} independently of each other. If the form of ϵ_{ij} is further simplified, many important network models are obtained as particular cases of eq.(3), including hidden-variable models, the configuration model and random graphs [6]. We shall introduce the temperature-dependent version of these models in what follows. We shall also exploit eq.(3) to study real networks and compute their temperature empirically. Therefore eq.(3) gives rise to a rich phenomenology and will be of central importance throughout the paper. Before considering its particular cases, let us first note some of its general properties. Note that, independently of T, $p_{ij} > 1/2$ when $\epsilon_{ij} < \mu$ and $p_{ij} < 1/2$ when $\epsilon_{ij} > \mu$. It is interesting to consider the infinite- and zero-temperature limits. When $T \to +\infty$ we have from eq.(3) that

$$p_{ij}(+\infty) = \frac{1}{2} \quad \forall i, j \qquad (4)$$

irrespective of the values of ϵ_{ij} and hence of the differences in the cost of links. As a consequence, the network is a random graph with $p = 1/2$ and is therefore trivial. Note that in this case any two configurations A and B become equiprobable ($P_A = P_B$). When $T = 0$ we have

$$p_{ij}(0) = \Theta(\mu - \epsilon_{ij}) \qquad (5)$$

so that only those pairs of vertices with $\epsilon_{ij} < \mu$ are connected. This is the well-known *degenerate* behaviour of Fermions at zero temperature, and μ is also termed the *Fermi energy* $\epsilon_F = \mu$. This clarifies the role of μ as the available energy per link when $T \to 0$: at absolute zero only the topology with the minimum value of $E_A - \mu L_A$ can be realized, and this topology is obtained by drawing all and only the links with $\epsilon_{ij} < \mu$. A final general comment is that eq.(3) reduces to the "classical" limit

$$p_{ij}(T) \approx e^{(\mu-\epsilon_{ij})/T} \qquad \text{when} \quad e^{(\epsilon_{ij}-\mu)/T} \gg 1 \qquad (6)$$

We now consider various specific cases. The simplest scenario is when all link energies are equal: $\epsilon_{ij} = \epsilon$. This yields a temperature-dependent random graph since all probabilities p_{ij} are equal to $p(T) = [e^{(\epsilon-\mu)/T} + 1]^{-1}$. While the properties of the random graph are well-known, in our framework some intriguing results emerge as $T \to 0$. First of all note that $p(0) = \Theta(\mu - \epsilon)$ and the graph is either fully connected ($\mu > \epsilon$) or empty ($\mu < \epsilon$). This provides us with a temperature-based definition of sparseness of a random graph: we can define a random graph as *sparse* (*dense*) if $\epsilon > \mu$ ($\epsilon < \mu$) since when $T = 0$ the graph becomes empty (fully connected). Then, it is clear that the critical probability $p_c \sim 1/N$ marking the percolation transition with the onset of a giant connected component can only be displayed by sparse graphs, and if we fix ϵ and μ with $\epsilon < \mu$ we can regard the phase transition as temperature-dependent. In particular, there is a *critical percolation temperature* T_c such that $p(T_c) = p_c \sim 1/N$. Inverting $p(T)$ we find

$$T_c = \frac{\epsilon - \mu}{\ln N} \to 0 \qquad N \to \infty \qquad (7)$$

Therefore when $N \to \infty$ we have the remarkable result that *the critical percolation temperature tends to zero, meaning that the zero-temperature topology naturally sets at the critical point $p = p_c$ and that at finite temperature the network is always above the percolation threshold.* This result is general: when the ϵ_{ij}'s are different we have $T_{min} \leq T_c \leq T_{max}$ where $T_{min} = (\epsilon_{min} - \mu)/\ln N \to 0$ and $T_{max} = (\epsilon_{max} - \mu)/\ln N \to 0$ as $N \to \infty$. Therefore $T_c \to 0$ in this case too, suggesting why large real world networks display a giant component. Interestingly, this behaviour is similar to a scenario explored in the theory of self-organized criticality (SOC) where the relation between a vanishing critical temperature and the onset of the SOC behaviour has been explored [11].

Another case of interest, showing the surprising effects of T, is when each link energy is the sum of two single-vertex contributions: $\epsilon_{ij} = \epsilon_i + \epsilon_j$. This is the grand-canonical version of the *configuration model* [6] since all graphs with the same degree sequence have the same E_A and are therefore equiprobable. The novelty of our

approach is that the *vertex fugacities* $x_i \equiv e^{-\epsilon_i/T}$ and $z \equiv e^{\mu/T}$ (in terms of which the model is conveniently described [12, 13]) now depend on T. We have

$$p_{ij}(T) = \frac{1}{e^{(\epsilon_i+\epsilon_j-\mu)/T}+1} = \frac{z x_i x_j}{1+z x_i x_j} \qquad (8)$$

The standard procedure to obtain scale-free degree distributions in this model is to assign each vertex i a fugacity x_i drawn from a power-law distribution $\rho(x) \sim x^{-\gamma}$ [12]. It has been shown that, since p_{ij} saturates to 1 as $x_i \to +\infty$, a cut-off appears in the degree distribution [12] ensuring that the degrees do not exceed N. This is for instance the case of the Internet [12] and of the World Trade Web (WTW) [13]. To highlight the role of T, it is interesting to rephrase these results in terms of the energies ϵ_i. For convenience we introduce the *vertex fitness* $\phi_i \equiv -\epsilon_i$ and we take it to be non-negative (this can always be achieved by a shift in the energies $\epsilon_i \to \epsilon_i - \epsilon_{max} \leq 0$). Therefore $\phi_i \geq 0$ (or $x_i \geq 1$) measures the tendency of vertex i to form connections [7]. Similarly, we define $\phi_0 \equiv -\mu$. Now, if we want x to be distributed according to $\rho(x) = (\gamma-1)x^{-\gamma}$ (where $1 \leq x < +\infty$ and $\gamma > 1$), then the fitness $\phi_i = -\epsilon_i = T \ln x_i$ must be distributed according to $q(\phi) = e^{-\phi(\gamma-1)/T}(\gamma-1)/T$. But since ϕ does not depend on T, $q(\phi)$ must be T-independent as well. The only possibility is therefore $(\gamma-1)/T = \lambda$ where λ is a constant independent of T. Without loss of generality we can reabsorbe λ in a rescaling of the energy $\epsilon \to \lambda\epsilon$ so that we can set $\lambda = 1$. This yields $\gamma = 1+T$ and

$$q(\phi) = e^{-\phi} \quad (\phi \geq 0), \quad \rho(x) = T x^{-1-T} \quad (x \geq 1) \qquad (9)$$

which is an important result showing how T determines $\rho(x)$ and consequently the topology of the network. For instance, in the classical limit (6) we recover the T-dependent version of a model studied in ref.[7]: since $p_{ij} \approx z x_i x_j$, the expected degree $\bar{k}_i = \sum_j p_{ij} \approx z x_i \sum_j x_j$ is proportional to x_i and is therefore distributed as $P(\bar{k}) \propto \bar{k}^{-1-T}$, but there are no degree correlations due to the factorization of p_{ij}. In the more general case, $P(k)$ has a power-law region with an exponent that is still an increasing function of T, followed by a cut-off due to the saturation of p_{ij}. The power-law region narrows as T increases. This qualitative behaviour can be characterized rigorously by computing $\bar{k}_i$ as a function of x_i or ϕ_i, and inverting this relation to find $P(\bar{k})$ from $\rho(x)$ or $q(\phi)$. This is not easy in general, but here we show that in the three paradigmatic cases $T = +\infty$, $T = 1$ and $T = 0$ it can be done successfully. For $T = +\infty$ we have the usual result $p_{ij} = 1/2$, and $P(\bar{k})$ approaches a trivial Poisson distribution with mean $N/2$. For $T = 1$, denoting $p_{ij} = p(\phi_i, \phi_j)$ we have

$$\begin{aligned} \bar{k} &= N\int_0^{+\infty} p(\phi,\phi')q(\phi')d\phi' = N\int_0^{+\infty} \frac{q(\phi')d\phi'}{e^{\phi_0-\phi-\phi'}+1} \\ &= N\frac{\ln(e^{\phi_0-\phi}+1)}{e^{\phi_0-\phi}} = Nzx\ln\frac{1+zx}{zx} \end{aligned} \qquad (10)$$

which is an increasing function of x and is therefore invertible, even if in a non-algebraic way. If $x(\bar{k})$ denotes the inverse function, the expected degree distribution is $P(\bar{k}) = \rho[x(\bar{k})]dx/d\bar{k}$. Note that $\bar{k} \propto x$ for small x, while $\bar{k} \to N$ for large x. Thus in the linear regime $x \propto \bar{k}$ while $dx/d\bar{k}$ is constant, implying $P(\bar{k}) \propto \rho[x(\bar{k})] \propto \bar{k}^{-2}$. This region is followed by a cut-off for large k corresponding to the saturated behaviour. Finally, when $T = 0$ the expression for $\rho(x)$ in eq.(9) breaks down since all the x_i's become infinite, and from eq.(5) we find

$$p_{ij}(0) = \Theta(\phi_i + \phi_j - \phi_0) \qquad (11)$$

Surprisingly, this coincides with another model introduced in ref.[7], which precisely assumes $q(\phi) = e^{-\phi}$ and thus turns out to be the zero-temperature limit of our general model. This model is intriguing since, using a derivation similar to that in eq.(10), it is shown [7, 8] to yield a purely scale-free degree distribution $P(\bar{k}) \propto \bar{k}^{-2}$ with no cut-off even if no power-laws are introduced "by hand" in it. Moreover, the model displays anticorrelation between degrees: the average nearest neighbour degree scales as $\bar{k}^{nn}(\bar{k}) \propto \bar{k}^{-1}$ and the clustering coefficient scales as $\bar{c}(\bar{k}) \propto \bar{k}^{-2}$ (times logarithmic corrections) [7, 8]. In our framework it is clear that ϕ_0 plays the role of a Fermi energy. We can also interpret the correlations at $T = 0$ as the collective need to minimise the total energy, an effect that gradually weakens as T increases. Taken together, these intriguing results show that in the above model *correlated scale-free networks with exponent -2 naturally arise as the zero-temperature optimized topology. As T grows, the correlations become weaker, the exponent of $P(\bar{k})$ increases and a cut-off appears in it destroying its purely scale-free behaviour, until for $T \to \infty$ the network becomes uncorrelated with a Poisson degree distribution.* If one has access to the empirical distribution $\rho(x)$, one can measure T for any real network which is well described by eq.(8). This is possible for the WTW, where x_i has been identified with the Gross Domestic Product of country i, whose distribution has a power-law tail with exponent -2 [13]. This means that $T_{WTW} = 1$ and that eq.(10) applies. This is consistent with the observed saturated behaviour of $k(x)$ and the cut-off displayed by $P(k)$ for the real WTW [13].

It is possible to further explore eq.(3) by considering different forms of $q(\phi)$ and of ϵ_{ij} as a function of ϕ_i and ϕ_j, thus recovering the whole class of hidden-variable models [7] with generic $p_{ij} = p(\phi_i, \phi_j)$. An even more general case is when ϵ_{ij} cannot be written as a function of single-vertex contributions, so that each pair of vertices has an associated *link fitness* $\phi_{ij} \equiv -\epsilon_{ij}$ drawn from a distribution $q(\phi)$, and a probability $p_{ij} = p(\phi_{ij})$ to exist. The range of possibilities is very broad, and among them we consider a particular case which allows for a direct application to real weighted networks and for the characterization of their temperature. Very recently [14] we explored the idea that the empirical weights w_{ij} in a real weighted network can be mapped into a matrix of probabilities $p_{ij} = p(w_{ij})$ defining an ensemble

Network	γ	T	Ref.
Metabolic flux networks	1.5	0.5	[15]
Interbank contract sizes	1.87	0.87	[16]
Erdős collaboration network	2	1	[17]
Chaos control & synchron. coauthorship	2.5	1.5	[17]
Financial cross-correlations	2.7	1.7	[18]
Financial cross-correlations	2.78	1.78	[19]
Financial cross-correlations	3.18	2.18	[19]
Mollusk research coauthorship	3.5	2.5	[17]
Unweighted graphs	$+\infty$	$+\infty$	

TABLE I: Empirical values of γ and T for weigthed networks.

of unweighted graphs, or *ensemble network*. In such a way, many topological properties which are non-obvious for weighted networks (such as the clustering coefficient) can be re-defined as ensemble averages of the corresponding unweighted quantities. In ref.[14] we explored the simplest possible choice where $p_{ij} \propto w_{ij}$. The results presented here suggest that this choice is the "classical" limit, equivalent to eq.(6), of a more general choice that we now consider. Turning to eq.(3), if we require $p_{ij} = 0$ when $w_{ij} = 0$ and $p_{ij} = 1$ when $w_{ij} = +\infty$, we find that w_{ij} must be proportional to the *link fugacity* $e^{-\epsilon_{ij}/T}$. In other words, the weights must depend on T, which corresponds to the property that at low T the least expensive links are the most exploited, while at high T all the weights are equal. Now, many real networks [15, 16, 17, 18, 19] display a power-law distribution of link weights $\rho(w) \propto w^{-\gamma}$ with $1.5 \leq \gamma \leq 3.5$ (see Table I). Therefore if we define $x_{ij} \equiv w_{ij}/w_{min} \geq 1$ (where w_{min} is the minimum nonzero weight for a given network), corresponding to the rescaling $\epsilon_{ij} \to \epsilon_{ij} - \epsilon_{max}$, we can repeat the arguments leading to eq.(9) and set $\epsilon_{ij} \equiv -T \ln x_{ij} \leq 0$ and $\phi_{ij} \equiv -\epsilon_{ij} \geq 0$ to obtain the same forms of $\rho(x)$ and $q(\phi)$. This allows us to compute the temperature of real networks with power-law distributed weights as $T = \gamma + 1$. The empirical values of γ found in various weighted networks [15, 16, 17, 18, 19] are summarized in Table I, and the corresponding values of T (ranging from 0.5 to 2.5) are also shown. By contrast, unweighted networks correspond to $T \to \infty$ where $x_{ij} = 1 \ \forall i, j$. We have therefore found that a general mapping from weights to probabilities in the context of ensemble networks is given by $p_{ij} = z x_{ij}/(1 + z x_{ij})$ where $x_{ij} \equiv w_{ij}/w_{min}$ and $z \equiv e^{\mu/T}$ is a free parameter. We note that the classical limit (6) of this expression reads $p_{ij} = z x_{ij}$, and if we choose $z = w_{min}/w_{max}$ we have $p_{ij} = w_{ij}/w_{max}$, which is approximately equivalent to the choice explored by us in ref.[14]. Turning to the full expression for p_{ij}, when $T \to 0$ eq.(5) implies that the original weighted network is mapped into a deterministic unweighted one where only the links with $\epsilon_{ij} < \mu$ are drawn. This means that the links with weight such that $x_{ij}(T) > z(T)$ in the limit $T \to 0$ are selected and the others are discarded. Interestingly, since the ordering of the weights is preserved at all temperatures, this corresponds to the threshold procedure adopted in ref.[20] to filter stock correlations and in ref.[21] to extract minimum spanning trees from real foodwebs. These filtering techniques discard most of the information contained in the weights, resulting in a single (threshold-dependent) unweighted graph. Here we find that this corresponds to the zero-temperature limit for an ensemble network. Our results allow us to apply these techniques to the finite temperature case in order to preserve the heterogeneity of the links and exploit it to obtain the whole ensemble of possible configurations.

We have presented a novel approach to complex networks by introducing the concept of temperature. We have shown many remarkable temperature-dependent effects resulting from topological optimization, and recovered several seemingly distinct models and techniques as particular cases of our unifying approach. This formalism gives an improved understanding of network topology and is open to further investigations.

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