Routes to thermodynamic limit on scale-free networks

Claudio Castellano¹ and Romualdo Pastor-Satorras²

¹SMC, INFM-CNR and Dipartimento di Fisica, "Sapienza" Università di Roma, P.le Aldo Moro 2, I-00185 Roma, Italy

²Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya, Campus Nord B4, 08034 Barcelona, Spain

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We show that there are two classes of finite size effects for dynamic models taking place on a scale-free topology. Some models in finite networks show a behavior that depends only on the system size N. Others present an additional distinct dependence on the upper cutoff k_c of the degree distribution. Since the infinite network limit can be obtained by allowing k_c to diverge with the system size in an arbitrary way, this result implies that there are different routes to the thermodynamic limit in scale-free networks. The contact process (in its mean-field version) belongs to this second class and thus our results clarify the recent discrepancy between theory and simulations with different scaling of k_c reported in the literature.

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The thermodynamic limit is a crucial concept in statistical physics. For example, no true singularity can occur in a system composed of a finite number N of elements at nonzero temperature [1], so that the very concept of phase-transition is well defined only in the limit $N \to \infty$. However, all real systems are finite, and more so in numerical simulations, and to study their properties one has to understand the role of finite size effects when the limit $N \to \infty$ is taken. In the case of critical phenomena, the theory of finite size scaling (FSS) [2] has successfully accomplished this task for processes on regular lattices, allowing to detect the signature of continuous phase-transitions even in very small systems. Finite size effects are expected to be all the more relevant for systems with a strongly heterogeneous interaction pattern, such as those described in terms of complex networks [3, 4]. Indeed, because of the small-world property [5] observed in most networks, the number of neighbors that can be reached starting from a certain node grows exponentially or faster with the geodesic distance. This implies that, even for large networks, just a few steps are sufficient to probe the finiteness of the system. Moreover, most real networks exhibit the scale-free (SF) property [3], i.e. they have a degree distribution P(k), defined as the probability that a vertex is connected to other k vertices, decaying for large k as $P(k) \sim k^{-\gamma}$ with $2 < \gamma \leq 3$, so that the local topological properties display very strong fluctuations, increasing with the size of the network [12]. In order to understand phase transitions, and in general any kind of dynamical process, in SF networks it is thus necessary to first comprehend how size effects, and in particular FSS, work in this class of systems.

Some attempts in this direction have been already done. For equilibrium continuous phase transitions the situations seems to be rather well established in some cases. For example, a FSS phenomenological theory has been developed for the Ising model [6, 8], based on a scaling ansatz for the free energy, leading to the FSS form for the magnetization at zero external field $m(\Delta, N) = N^{-\beta/\bar{\nu}} f(\Delta N^{1/\bar{\nu}})$, where Δ is the distance to the critical point, and the critical exponents β and $\bar{\nu}$ depend on the degree exponent γ and are defined only for $\gamma > 3$ [22]. In the context of nonequilibrium phase transitions, however, the situation is not so clear. In the case of the contact process (CP) in SF networks [7] Hong *et al.* [8] proposed a FSS for the average density of particles in surviving runs scaling as $\rho_s(\Delta, N) = N^{-\beta/\bar{\nu}} f(\Delta N^{1/\bar{\nu}})$, with $\beta = 1/(\gamma - 2)$, $\bar{\nu} = (\gamma - 1)/(\gamma - 2)$ for $2 < \gamma \leq 3$, and $\beta = 1$, $\bar{\nu} = 2$ for $\gamma > 3$. This theory, however, is still under debate [9, 10], since numerical simulations in random neighbors SF networks yield incompatible results [10]. For other kinds of FSS, see also Ref. [11].

In this Letter we provide a step forward in the understanding of finite size behavior in dynamical processes on SF networks by showing that two different scaling scenarios may occur. A first class of processes exhibits finite size effects depending exclusively on the network size N. On the other hand, a second class of processes displays anomalous finite size effects, in the sense that their properties depend explicitly and independently not only on the number of nodes N, but also on the upper cutoff k_c of the degree distribution [12]. Hints to this fact can be found in previous works in which explicit solutions for dynamical models on SF networks with infinite size but finite cutoff were obtained [13]. In this case, an explicit dependence on k_c was found, leading to a radically different behavior from that obtained for truly infinite SF networks, which then do not correspond to the analytical continuation to infinite k_c . The true thermodynamic limit of SF networks corresponds to the double limit $N \to \infty$ and $k_c \to \infty$, since keeping k_c fixed leads to a finite degree second moment even for $\gamma < 3$, and to a non SF network. The natural way to take this double limit is to allow k_c to diverge with N but not faster than $N^{1/2}$ if the network is to be uncorrelated [14]. Hence any choice $k_c(N) \sim N^{1/\omega}$ with $2 \leq \omega < \infty$ is legitimate and the way to reach the thermodynamic limit is not

unique. Therefore, in systems with anomalous finite size effects, depending on the way k_c scales with system size, the final behavior as a function of N is modified, and will depend on the particular value of ω chosen. The heterogeneous mean-field (MF) theory for CP turns out to display anomalous scaling, therefore our findings clarify the discrepancies between MF theory and random-neighbor simulations recently reported in the literature [10]. More generally, our results indicate that the FSS analysis with the standard form (i.e. as a function of N alone) used in several recent works for SF quenched networks should be reconsidered.

We start our case by considering the contact process [15] on heterogeneous networks, which is defined as follows [7]. An initial fraction ρ_0 of vertices is randomly chosen and occupied by a particle. Dynamics evolves in continuous time by the following stochastic processes: Particles in vertices of degree k create offsprings into their nearest neighbors at rate λ/k , independently of the degree k' of the nearest neighbors. At the same time, particles disappear at a unit rate [23]. This model undergoes a continuous transition, located at a critical point λ_c , separating an absorbing phase from an active one with everlasting activity [15]. The critical properties of CP on uncorrelated SF networks have been studied by means of heterogenous MF theory [7] and a FSS theory [8]. Heterogeneous MF theory predicts in the thermodynamic limit a critical point $\lambda_c = 1$, independent of the network topology, a stationary particle density in the active phase given by $\rho \sim \Delta^{\beta}$, with $\Delta = \lambda - \lambda_c$ and $\beta = 1/(\gamma - 2)$, and a density decay at criticality $\rho(t) \sim t^{-\theta}$, with $\theta = 1/(\gamma - 2)$. On the other hand, Ref. [8] assumes a standard FSS, depending only on N, which yields the particle density in surviving runs at criticality

$$\rho_s \sim N^{-1/(\gamma - 1)},\tag{1}$$

for any $k_c > N^{1/\gamma}$. Apart from the unsolved question of the validity of heterogeneous MF theory for CP on uncorrelated SF networks [7, 9, 10], there is surprising evidence of a disagreement between the MF FSS exponents and simulations on a random neighbor version of SF networks [10]. In order to gain an understanding of finite size effects in the CP, we propose to focus on spreading experiments [15], i.e. in simulations starting with a single active site ($\rho(t = 0) = \rho_0 = 1/N$) in which activity is followed until the systems decays to the absorbing state. In such experiments it is customary to measure the survival probability P(t), defined as the probability that activity survives up to time t. At the critical point this quantity scales as [15]

$$P(t) = t^{-\delta} f(t/t_c), \qquad (2)$$

where the scaling function f(x) is constant for small values of the argument and cutoff exponentially for $x \gg 1$,

and t_c is a characteristic time, depending usually on the size of the system. Standard homogeneous MF FSS theory predicts that at criticality the temporal cutoff scales as $t_c \sim N^{1/2}$ [15]. To gain insight into the spreading experiment, we can map the dynamics at the MF level onto an effective one-dimensional diffusion problem. When a spreading experiment for the CP is performed the number of active sites n(t) starts at 1 and at each time step can grow by 1, decrease by 1 or remain constant. Defining the density of active sites $\rho(t) = n(t)/N$, the diffusion process is defined in uncorrelated networks at criticality by the transition rates

$$\omega_{\rho \to \rho - \frac{1}{N}} = \rho(t), \ \omega_{\rho \to \rho + \frac{1}{N}} = \rho(t) \sum_{k} \frac{P(k)k}{\langle k \rangle} [1 - \rho_k(t)],$$
(3)

where the last term in Eq. (3) represents the probability that a random neighbor is empty, and $\rho_k(t)$ is the density of active sites restricted to nodes of degree k. Clearly $\rho(t) = \sum_k \rho_k(t) P(k)$. The equation of motion for the ρ_k at criticality is [7]

$$\partial_t \rho_k(t) = -\rho_k(t) + \frac{k}{\langle k \rangle} [1 - \rho_k(t)] \rho(t).$$
(4)

Since all ρ_k are expected to change in time slower than exponentially, it is correct to perform a quasi-static approximation [16] and set the l.h.s. of Eq. (4) to zero, so that

$$\rho_k(t) \simeq \frac{k\rho(t)/\langle k \rangle}{1 + k\rho(t)/\langle k \rangle} \tag{5}$$

at sufficiently large times. Provided $\rho(t) \ll \langle k \rangle / k$, which is always true in spreading experiments, the k-dependent term in the denominator can be neglected, i.e. $\rho_k(t) \simeq k\rho(t)/\langle k \rangle$. This relation is very well verified numerically. Inserting it into the transition rates yields

$$\omega_{\rho \to \rho - \frac{1}{N}} = \rho(t), \quad \omega_{\rho \to \rho + \frac{1}{N}} = \rho(t) \left[1 - g\rho(t)\right], \quad (6)$$

where $g = \langle k^2 \rangle / \langle k \rangle^2$. Hence the density $\rho(t)$ of active states performs a biased, one-dimensional random walk, and the distribution Eq. (2) is the solution of the first passage time problem in $\rho = 0$, starting from the initial condition $\rho_0 = 1/N$. Using the transitions rates (6) it is possible to measure the time t_c with arbitrary precision in trivial simulations of the random walk process. It turns out that this characteristic time depends explicitly on both the network size N and the network cut-off k_c , through the form

$$t_c \sim \left(N/g\right)^{1/2}.\tag{7}$$

For $\gamma > 3$, (non SF networks), g is a constant and Eq. (7) coincides with the usual MF result. For $\gamma \leq 3$, on the other hand, g diverges with the upper cutoff k_c of the degree distribution as $k_c^{3-\gamma}$, giving an anomalous form of

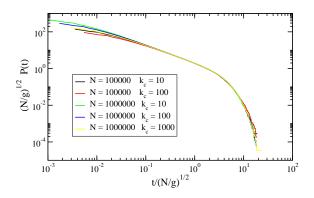


FIG. 1: Scaling plot of the survival probability of the CP on random neighbors SF networks with $\gamma = 2.5$ and $k_c \leq N^{1/2}$. Minimum degree $k_{\min} = 2$. Numerically we obtain $\delta = 1$.

FSS, which separately and explicitly involves the system size N and the cutoff k_c , i.e.

$$t_c \sim N^{1/2} k_c^{(\gamma-3)/2}.$$
 (8)

We have verified numerically, by performing spreading experiments on a random neighbors version of the uncorrelated configuration model [17] with $k_c < N^{1/2}$, that the surviving probability of the CP at criticality is well described by Eq. (2) with a characteristic time t_c given by Eq. (7), see Fig. 1. As we have discussed above, the cutoff k_c is not fixed, and its divergence with network size can be chosen with a degree of arbitrariness. Imposing therefore $k_c(N) \sim N^{1/\omega}$ and expressing t_c only as a function of N, this arbitrariness results in a dependence on the exponent ω ,

$$t_c \sim N^{[1+(\gamma-3)/\omega]/2}$$
. (9)

This anomalous dependence of t_c on both N and k_c translates into a density of active sites in surviving runs ρ_s (the usual observable for FSS in non-equilibrium absorbingstate phase transitions) depending also separately on Nand k_c . To determine its detailed expression, it is crucial to realize that the solution of the MF Eq. (4) for $\rho(t)$ at criticality shows a crossover at a temporal scale $t^* \sim k_c^{\gamma-2}$, in full analogy with the crossover occurring for diffusion-annihilation processes in SF networks [16]. The origin of the crossover can be traced back to Eq. (5). When there is a finite initial density ρ_0 of active sites, the k-dependent term in the denominator of Eq. (5) cannot be neglected and hence, for $t_{\times} < t < t^*$, the density decays as if the network size were effectively infinite, so that $\rho(t) \sim t^{-1/(\gamma-2)}$ [7]. t_{\times} is a microscopic time scale, independent of N and k_c . As the density decreases, for times larger than t^* , such that $k_c \rho(t^*) = \langle k \rangle$, the denominator of Eq. (5) does not effectively depend on k anymore so that for $t^* < t < t_c$, $\rho(t) \sim (gt)^{-1}$ for any γ , yielding an exponent $\theta = 1$. The asymptotic value in surviving runs ρ_s is reached for times larger than t_c , so $\rho_s \sim \rho(t_c)$.

Since $t_c > t^*$ for $\gamma < 3$ and $\omega > 2$, one has at the critical point

$$\rho_s \sim \frac{1}{gt_c} \sim N^{-1/2} k_c^{(\gamma-3)/2} \sim N^{-[1-(\gamma-3)/\omega]/2}.$$
 (10)

Eq. (10) shows that not only t_c but also other observables acquire an anomalous k_c -dependence on finite SF networks, which translates into values of the exponent ratio $\beta/\bar{\nu}$ depending on the particular ω considered. This result accounts for the numerical difference in the $\beta/\bar{\nu}$ value found in random neighbor simulations with different values of ω [10], which can be better fitted [24] by means of Eq. (10), whose decay exponent is smaller than the one proposed in Refs. [8, 9], namely Eq. (1). It is also worth stressing that, since $t_c > t^*$, the true asymptotic MF value for the temporal exponent θ describing the decay of density is 1 for any γ and any $N < \infty$, and not the exponent $1/(\gamma - 2)$ predicted for $\gamma < 3$ by the heterogeneous MF treatment for strictly infinite system size [8, 9].

This finite size separate dependence of scaling time at criticality on both the system size and the upper cutoff is not in fact a peculiarity of the CP in MF, but is actually found also in other processes taking place on SF networks. Sood and Redner [18] have recently computed the time needed by the voter model dynamics taking place on heterogeneous networks to reach a full consensus (ordered) state, which is given by $\tau \sim N/q$, and hence depends on both N and k_c for $\gamma \leq 3$. On the other hand, the distinct dependence on N and k_c is not the only possibility: There are systems for which the size scaling on heterogeneous networks is not anomalous and depends exclusively on N. Two examples are provided by the "link-update" [19] and "reverse" [20] versions of the voter model. In the first case the time to reach full consensus is proportional to N [20], with no dependence on network features whatsoever. For the reverse model instead such time is proportional to $N\langle k\rangle\langle k^{-1}\rangle$ [20]. For all $\gamma > 2$ these moments of the degree distribution are well-behaved and no dependence on k_c arises. In this same spirit, it is possible to devise stochastic systems with continuous phase transitions that show standard finite size effects, depending only on the network size. Consider, for example, the variation of the CP proposed in Ref. [21] (see also [11]) in which particles in vertices of degree k create offsprings in nearest neighbors of degree k' at rate $\lambda(kk')^{-\mu}$, while particles still disappear at unit rate. For $\mu = 1$, the heterogeneous MF theory for this model takes, in uncorrelated networks, the form

$$\partial_t \rho_k(t) = -\rho_k(t) + \frac{\lambda \rho(t)}{\langle k \rangle} [1 - \rho_k(t)], \qquad (11)$$

which has a threshold $\lambda_c = \langle k \rangle$, and a stationary particle density in the active phase $\rho \sim \lambda - \lambda_c$. It is easy to see that the random walk mapping of spreading experiments

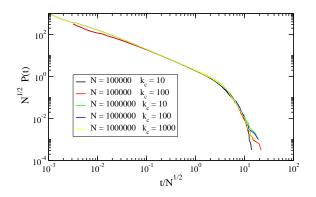


FIG. 2: Scaling plot of the survival probability of the modified CP in Ref. [21] with $\mu = 1$, on random neighbors SF networks with $\gamma = 2.5$ and $k_c \leq N^{1/2}$. Minimum degree $k_{\min} = 2$.

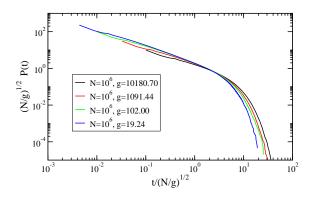


FIG. 3: Scaling plot of the survival probability of the CP on random neighbors SF networks with $\gamma = 2.5$ and $k_c = N^{1/(\gamma-1)}$. Minimum degree $k_{\min} = 2$. Notice that, for $\omega < 2$, g displays very large sample to sample fluctuations.

at criticality in this modified CP model is defined by the transition rates in Eq. (6) with g = 1, which correspond to a characteristic time scaling as $t_c \sim N^{1/2}$, completely independent of the network cutoff k_c . This result is fully confirmed by numerical simulations, see Fig. 2.

Finally, let us discuss what happens in the standard CP when the cutoff scales as $k_c \sim N^{1/\omega}$ but with $\omega < 2$. This case includes the so-called natural cutoff $\omega = \gamma - 1$ (for $\gamma < 3$) that occurs in the configuration model if one does not impose any constraint on the maximum degree of the vertices [12, 14]. In such a case, the presence of very large hubs invalidates the derivation of the Eq. (7). Figure 3 shows that this is in fact the case for $\gamma < 3$ and $\omega = \gamma - 1 < 2$, and it is then the proof that for random neighbor networks with $k_c > N^{1/2}$ a different scaling form of t_c must be considered.

In conclusion, the evidence presented in this work leads to the conclusion that processes taking place on SF networks may be divided in two classes. In the first class, finite size effects and FSS depend only on the number of nodes N. This class encompasses "reverse" and "linkupdate" voter dynamics as well as models showing continuous phase transitions, such as the Ising model for $\gamma > 3$, and modified versions of the CP. Other models, on the other hand, show an additional explicit dependence on the upper cutoff of the degree distribution. In this last case the thermodynamic limit of an infinitely large network can be reached in different ways, depending on how k_c is chosen to scale with N, and different possible routes to the thermodynamic are thus possible. Understanding what physical ingredients select which class a model belongs to is a challenging task for future work.

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- no meaning in this region. [23] For a discrete time implementation of this model, see Ref. [7].
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