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Method to estimate critical exponents using numerical studies

E. Perlsman and S. Havlin

Minerva Center and Department of Physics, Bar-Ilan University
52900 Ramat-Gan, Israel

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Abstract. – A novel method to estimate the critical point and critical exponents of physical models from numerical studies is presented. The method utilizes linear approximation to compute the values of the characteristic variables in the near vicinity of the critical point from numerical results obtained for only one point in that vicinity. The method is applied to two models: Two-dimensional directed percolation, and one-dimensional reaction-diffusion model. In both cases the critical point and critical exponents are determined with higher accuracy than achieved in former studies. In the reaction-diffusion model, the results strongly suggest simple rational values of 1/3, 1/12, etc., for the characteristic exponents.

The estimation of critical exponents of various models from numerical studies is a task which frequently occurs in statistical physics and phase transitions. Different simulation algorithms have been applied to various models, and no method is considered superior to others. This article presents a new method to perform the task, and describes its application to two different models: Two-dimensional directed percolation, and the reaction-diffusion model introduced in [1] and numerically studied in [2]. The results obtained for these models suggest that this method might be successfully applied to a large class of models of critical phenomena. The study also suggests simple rational values for the exponents in the reaction-diffusion model.

The article starts with the presentation of the method, and follows by the presentation of the numerical results obtained for the two models.

The models which are referred to in this study are characterized by the following relation: $V(q_c, t) \sim t^e$, where V is a dependent variable, q is an independent state variable, q_c is the critical point at which the above relation holds, t is the time or space variable, and e is the critical exponent considered. The models are characterized by some type of random process, and numerical simulations are performed in order to estimate the values of q_c and e.

The common approach to this estimation task is to perform numerical simulations for various values of q, and to find the value of q for which the log-log plot of $V(q, t)$ *vs.* t is a straight line. However, this search procedure consumes a lot of computer time, and the more precise the value of q_c to be determined, the longer the search procedure. Moreover, usually

the simulations should be performed up to large values of t, because the relation $V(q_c, t) \sim t^e$ is not revealed at small values of t, due to finite-size effects.

The estimation method used in this study is based on the ability to search for q_c using numerical results obtained for only a single value of q (denoted by q_0). After the estimation of $V(q_0, t)$ is performed, the value of $V(q, t)$ for any other q is computed by a linear extrapolation from $V(q_0, t)$ to $V(q, t)$.

The use of linear approximation near the critical point is based on the following relation [3, 4]:

$$V(q,t) \simeq V(q_c,t)\big(1 + ct^{1/\nu_t}(q - q_c)\big). \tag{1}$$

In eq. (1), c is a constant, and ν_t is determined by the relation: $\xi \sim |q - q_c|^{-\nu_t}$, where ξ is the characteristic length (or time) scale of the system at q. Equation (1) implies that for fixed t values, and small enough Δq, the graph of $V(q)$ *vs.* q is a straight line whose slope is $V(q_c, t)ct^{1/\nu_t}$.

Suppose now that we have an estimate of $V(q, t)$ at a specific point q_0, and we want to check whether another point, q_1, is the critical point. If q_1 is the critical point, then $V(q_0, t) \simeq V(q_1, t)(1 + ct^{1/\nu_t}(q_0 - q_1))$, and thus

$$V(q_1,t) \simeq V(q_0,t)/\big(1 + ct^{1/\nu_t}(q_0 - q_1)\big). \tag{2}$$

Having estimates of $V(q_0, t)$, c and ν_t, we can thus compute the estimate of $V(q_1, t)$, and check whether the log-log plot of $V(q_1, t)$ *vs.* t is a straight line. Of course, q_0 should be close enough to q_c so that the linear approximation is valid.

The estimation procedure is thus performed by the following steps:

1. Obtain numerical results for moderate t values and various q values. From the numerical results obtained at this stage get estimates of q_c, ν_t and c.

2. Obtain one set of numerical results for $V(q_0, t)$, where q_0 is the value of q_c estimated at the first stage. This set is obtained up to the largest reasonable values of t. Naturally, most of the computer time is invested at this stage.

3. Use the estimates of c, ν_t and $V(q_0, t)$ obtained in stages 1 and 2 to compute $V(q_1, t)$ at various q_1 values using eq. (2). The value of q_1 at which the log-log plot of $V(q_1, t)$ *vs.* t yields a straight line is the new estimated q_c, and the slope of this straight line is the estimate of the corresponding exponent e. It should be noted that possible inaccuracies in the estimates of c and ν_t have only second-order effects on the estimates of q_c and e.

In this study the numerical results are presented in terms of local values of the exponent e computed as $\log_{m^2}(V(q, mt)/V(q, t/m))$, where m is a constant which was assigned with the values 2 or 4. The local values of the exponent express the slope of the log-log plot of $V(q, t)$ *vs.* t, and the demand that this plot yields a straight line is equivalent to the demand that the local values of e arrive at their asymptotic value.

The above-presented method is demonstrated in the following for two models: Two-dimensional $(2 + 1)$ directed-percolation, and one-dimensional reaction-diffusion model.

In the directed-percolation model [5], the bonds (or sites) of a lattice are assigned at random with the values 0 or 1. A zero-valued bond connects two sites in a predefined direction, while a one-valued bond disconnects them. The connected sites form a directed-percolation cluster. The simulations for the model were performed on a random bond BCC lattice, and the directed-percolation clusters were grown using the Leath method [6]. The directed-percolation model can be characterized by the following relations: $N(p_c, t) \sim t^\alpha$; $n(p_c, t) \sim t^{-\delta}$. Here,

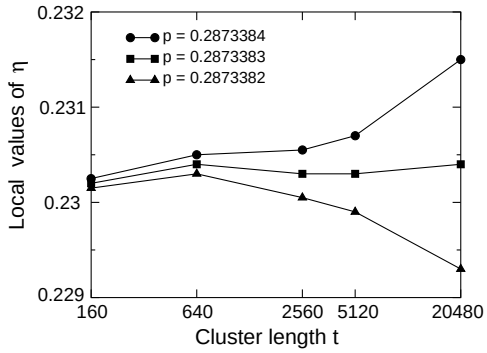

Fig. 1

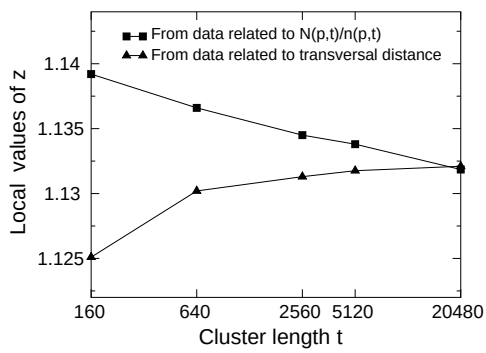

Fig. 2

Fig. 1 – The local values of the exponent η as a function of the cluster length. The results are presented for three bond probabilities: 0.2873384, 0.2873383 and 0.2873382. The three curves in this figure are computed from the same set of numerical results obtained for $p = 0.2873380$, and extrapolated to the relevant probabilities using eq. (2).

Fig. 2 – The local values of the exponent z as a function of the cluster length. The results are computed from two independent sets of data: The upper curve from data related to the quotient $N(p,t)/n(p,t)$, thus giving the sum of α and δ. The lower curve from data related to the mean-squared transversal distance of the sites of the base from the origin.

$N(p,t)$ is the number of sites in the t layer of the directed-percolation cluster, $n(p,t)$ is the percentage of clusters which survive the growth process up to length t, and p is the probability that the random bonds are assigned with the value 0. The product and quotient of $N(p,t)$ and $n(p,t)$ determine two other growth exponents: $N(p_c,t) \cdot n(p_c,t) \sim t^{\eta}$, with $\eta = \alpha - \delta$, and $N(p_c,t)/n(p_c,t) \sim t^{z}$, with $z = \alpha + \delta$. In this model the characteristic length scale (or longitudinal correlation length) is usually denoted by $\xi_{\parallel} \sim \Delta p^{-\nu_{\parallel}}$, and since the model is asymmetric, it has a different characteristic transversal length scale: $\xi_{\perp} \sim \Delta p^{-\nu_{\perp}}$. A scaling relation which holds between the exponents is $z = d\nu_{\perp}/\nu_{\parallel}$, where d is the dimension of the layers of the lattice ($d = 2$ in the present case).

The estimation procedure followed the steps described above. At the first stage numerical results for $n(p,t)$ and $N(p,t)$ were obtained for p values in the vicinity of 0.287338 (the estimated p_c of ref. [4]). The slopes of the graphs of $n(p)/n(p_c)$ and $N(p)/N(p_c)$ *vs.* p were computed for $t = 1280$ and $t = 5120$. From these slopes the estimates of c and $\nu_{\parallel}$ were obtained. Naturally, $N(p,t)$ and $n(p,t)$ are characterized by different values of c, but $\nu_{\parallel}$ is identical in both cases.

At the second step of the estimation procedure, directed-percolation clusters were grown at $p = 0.287338$ up to length $t = 81920$, and the variables $N(t)$ and $n(t)$ were estimated. More than 100000 clusters were grown at each length.

At the third step, the results of the first two steps were combined in order to search for p_c. The results of the search indicated that the local values of α, δ and z do not exhibit asymptotic behaviour in the range of t values studied. Only for η it was possible to find a value of p in which the last local values of the exponent exhibit asymptotic behaviour. Figure 1 presents the local values of η for three probabilities: 0.2873382, 0.2873383, 0.2873384. For $t \leq 2560$, m was taken as 2, while the last two local values of the exponent were computed with $m = 4$. It should be emphasized that the three curves presented in the figure are based on the same set of numerical results obtained for $p = 0.2873380$, and extrapolated to the relevant probabilities

using eq. (2). The central curve of this figure, which is related to $p = 0.2873383$, presents five local values with a difference of 0.0003 between their minimum and maximum. These results enable estimation of p_c at 0.2873383(1), and the estimate of η is 0.2303(4). As can be clearly seen in this figure, the estimate of η could be derived from the results obtained for smaller clusters, and the role of the last two local values of the exponent is to enable determination of p_c with enhanced accuracy. The estimated value of p_c is determined by the demand that the last local values of η, computed at p_c, are found in the vicinity of 0.2303.

As noted above, from scaling relations there follows the identity $2\nu_\perp/\nu_\parallel = z = \alpha + \delta$. The value of $\nu_\perp/\nu_\parallel$ is the roughness exponent usually denoted by ν, and the mean-square transversal distance of the sites of the t layer from the origin should grow proportional to $t^{2\nu}$. The local values of $z = 2\nu$ computed in this way are compared in fig. 2 with those obtained from the data related to the quotient $N(p,t)/n(p,t)$, which gives the sum of the local values of α and δ. As can be seen, only for $t = 20480$ the two sets of local values are met with a difference which is smaller than their error ranges. The combination of these two independent estimates yields an estimate for z at 1.1321(6).

From this estimate of z, combined with the above-presented estimate of $\eta = 0.2303(4)$, and with the aid of the scaling relations $2\delta = z - \eta$; $2\alpha = z + \eta$, the following estimates are obtained: $\delta = 0.4509(5)$ and $\alpha = 0.6812(5)$. Since the local values of z, computed in both ways, are almost insensitive to a slight change in p, it is the data related to η, presented in fig. 1, which determines all the other estimates including the one for p_c.

A comparison of the above results with those of former publications [4, 7, 8], reveals two main advantages of this study:

1. The critical probability p_c is determined to an accuracy which is more than an order of magnitude higher than the former estimation presented in [4].

2. In the three former publications [4, 7, 8], the difference between the sum of the best estimates of α and δ, and the independent estimate of z, is 0.002, while in this study the difference between the two independent estimates is only 0.0003, almost an order of magnitude smaller than the former discrepancies. This fact enables the presentation of consistent estimates for all the four characteristic exponents.

The second model for which the above estimation method was applied is a reaction-diffusion model described in [1,2]. This model refers to two types of particles: type A and type B. Both types of particles perform a random walk along a one-dimensional lattice. When an A particle meets a B particle it transforms into a B particle, and at each time step, the B particle has a fixed probability to spontanously transform into an A particle. The total density of particles is denoted by ρ, and the density of B particles is denoted by ρ_B. It should be noted that ρ is conserved, and thus, $\rho_A = \rho - \rho_B$, where ρ_A is the density of A particles. In a low total density, the steady state is a state with only A particles, while for high total density and an initial condition with the presence of B particles, the steady state is a state with fixed ρ_A and ρ_B. The transition from a steady state with $\rho_B > 0$ to a steady state with $\rho_B = 0$ occurs at the critical (total) density ρ_c.

At the critical density ρ_c, a system with the presence of B particles can evolve in time by two different modes of time dependence, which depend on the initial conditions. If $\rho_B(\rho_c, 0)$ is high, ρ_B will uniformly decrease towards zero following the (asymptotic) relation $\rho_B(\rho_c, t) \sim t^{-\delta}$. If $\rho_B(\rho_c, 0)$ is low, ρ_B will increase at first following the (quasi-asymptotic) relation $\rho_B(\rho_c, t) \sim t^{\eta}$, and after some time (which depends on the initial conditions), it starts to decay towards zero following the (asymptotic) relation $\rho_B(\rho_c, t) \sim t^{-\delta}$. Starting a system with the presence of a single B particle, the exponents α, δ, η and ν have similar meanings to those associated earlier

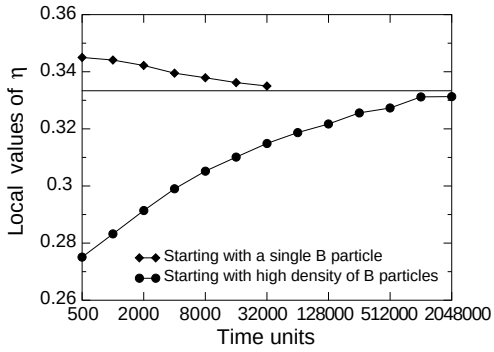

Fig. 3 – The local values of the exponent η as a function of time for $\rho = 0.2776$. The upper curve is computed directly from numerical results obtained for systems which start with the presence of a single B particle. The lower curve is computed indirectly using the relation $\eta = 0.5 - 2\delta$, and the local values of δ were obtained for systems with high initial ρ_{B}. In order to ease comparison between the two data sets, a horizontal line at the value of $\eta = 1/3$ is added to the figure.

with the directed percolation model. Since the system studied is one dimensional, the scaling relation is $\alpha + \delta = \nu$.

It should be noted that the notation used in refs. [1, 2] is different from the notation used in this article, and in order to avoid confusion, it is necessary to clarify the relations between the two sets of notations: Their ν is our $\nu_{\perp}$, their z is our $1/\nu$, and their η is our $-\eta/\nu$.

In [1, 9] it was shown that $\nu = 1/2$ ($z = 2$ in their notation). Since ν is known, and since the scaling relation $\alpha + \delta = \nu$ is valid in this case, there is only one independent exponent in the set α, δ, η. Thus, an estimate of one of them supplies us with estimates for the other two.

The estimation procedure was performed for the the two modes of time dependence, and followed the same steps described above for directed percolation. Naturally, the critical density ρ_{c} depends on the random walk probabilities, and on the probability of a B particle to spontanously transform into an A particle. In order that our estimate for ρ_{c} will be comparable to the one presented in [2], these probabilities were assigned with the same values assigned to them in [2]. The results were obtained at $\rho = 0.277$, and extrapolated to the different ρ values using eq. (2). Since the numerical simulations for the two modes of time dependence have different computer time demands, the results for the systems which start with high ρ_{B} values were obtained for $t \leq 4096000$, while those for the systems which start with a single B particle were obtained only for $t \leq 64000$.

The results of the first set (high initial ρ_{B}) supply a direct estimate for δ, while those of the second set (starting with a single B particle) supply direct estimates for all the four exponents. In order to compare the estimates obtained from the two sets of numerical results, fig. 3 presents the local values of η estimated from these two sets. (Note again that our η is $-\eta/2$ in the notation of [1, 2].) The upper curve of this figure presents direct estimates of the local values of η obtained from the second set (starting with a single B particle). The lower curve presents indirect estimates of the local values of η computed from the relation $\eta = 0.5 - 2\delta$, where the local values of δ were estimated from the results of the first set (high initial ρ_{B}). The results are presented for the estimated ρ_{c}, $\rho = 0.2776$, and the local values of the exponents are computed using $m = 2$.

As can be seen in fig. 3, both sets of local values approach similar asymptotic values. It is interesting to note that just like in the directed-percolation case, in this case also the local

values of η present convergence to an asymptotic value at much lower t values than those of δ (from which the lower curve of fig. 3 was drawn). However, unlike the picture presented in fig. 1, no curve in fig. 3 presents asymptotic behaviour at this range of t values. Thus, it is only the combination of the two data sets which enable estimation of ρ_c and η with relatively low error ranges. Since the gap between the last points of the two data sets is 0.003, the resultant estimate of η is $\eta = 0.333(4)$. Taking into account the sensitivity of the local values of the exponents to a change in p, the estimate of p_c is $p_c = 0.2776(2)$. It should also be noticed that in the present case, the estimates of ρ_c and η are not independent: a higher estimate of ρ_c is associated with a higher estimate of η.

The estimate of $\eta = 0.333(4)$, combined with the known value of $\nu = 0.5$, supply a strong indication for rational values of 1/3, 1/12, 5/12 of the exponents η, δ and α, respectively. A comparison of these estimates to those presented in [2] reveals significant discrepancies, which are mainly a result of the higher estimate of ρ_c in our study. The long duration of finite-size effects, demonstrated in the lower curve of fig. 3, might be the reason for these discrepancies.

In conclusion, this article presents a simple method for the estimation of the critical constants from numerical simulations. The estimates which were obtained using this method are significantly better than those obtained using other methods, a fact which suggests that this method might be applied to a large class of models.

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