# Reweighting in nonequilibrium simulations

Ronald Dickman*

*Departamento de Física, Universidade Federal de Santa Catarina, Campus Universitário Trindade, CEP 88040-900, Florianópolis, SC, Brazil*

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A simple reweighting scheme is proposed for Monte Carlo simulations of interacting particle systems, permitting one to study various parameter values in a single study, and improving efficiency by an order of magnitude. Unlike earlier reweighting schemes, the present approach does not require knowledge of the stationary probability distribution, and so is applicable out of equilibrium. The method is applied to the contact process in two and three dimensions, yielding the critical parameter and spreading exponents to unprecedented precision. [S1063-651X(99)50607-7]

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Reweighting and histogram methods, which permit one to calculate thermal averages at different temperatures from a single sample, have greatly improved the efficiency of Monte Carlo simulations [1]. Given a sample of configurations, $C_1, \ldots, C_N$, generated at temperature $T$, one can in principle generate a sample appropriate to some temperature $T'$, by assigning the weight $w_i = P_i(T')/P_i(T)$ to configuration $i$. Until now, such methods have been restricted to equilibrium, where the stationary probability distribution is $P_i \propto e^{-E_i/kT}$. Away from equilibrium, one does not in general know the stationary distribution, so there is no simple way to evaluate the $w_i$. Recently Grassberger and Zhang showed how a ''self-organized'' formulation of directed percolation can be used to study several parameter values in a single run, without reweighting [2]. In this work I introduce a reweighting scheme for interacting particle systems, based on the observation that, despite our ignorance of the *stationary* distribution on configuration space, we can write down the probability for any sequence of events between time zero and time $t$.

I apply the reweighting method to the contact process (CP), a simple particle system (lattice Markov process) exhibiting a phase transition to an absorbing (frozen) state at a critical value of the creation rate [3]. This model belongs to the universality class of directed percolation [4] and Reggeon field theory [5] (it is one of the most well-studied representatives of this class [6]), and is pertinent to models of epidemics [7], catalysis [8], and damage spreading [9]. In the CP each site of the hypercubic lattice $\mathcal{Z}^d$ is either vacant or occupied by a particle. Particles are created at vacant sites at rate $\lambda n/2d$, where $n$ is the number of occupied nearest neighbors, and are annihilated at unit rate, independent of the surrounding configuration. The order parameter is the particle density $\rho$; the vacuum state, $\rho = 0$ is absorbing. As $\lambda$ is increased beyond $\lambda_c$, there is a continuous phase transition from the vacuum to an active state; for $\lambda > \lambda_c$, $\rho \sim (\lambda - \lambda_c)^\beta$ in the stationary state.

There are a number of ways (equivalent as regards scaling behavior) of implementing the CP in a simulation algorithm; in this work I follow the widely used practice of maintaining a list of all occupied sites. Trials begin at time zero, from a fixed initial configuration. Subsequent events involve selecting (at random) an occupied site $\mathbf{x}$ from the $N_p$ sites on the list, selecting a process: creation with probability $p = \lambda/(1+\lambda)$, annihilation with probability $1-p$, and, in the case of creation, selecting one of the $2d$ nearest neighbors, $\mathbf{y}$, of $\mathbf{x}$. (The creation attempt succeeds if $\mathbf{y}$ is vacant.) The time increment $\Delta t$ associated with an event is $1/N_p$, where $N_p$ is the number of occupied sites immediately prior to the event. A trial ends when all the particles have vanished, or at the first event with time $\geq t_m$, a predetermined maximum time.

Consider a single trial, extending from time zero up to $t_m$; for simplicity, suppose that initially there is but a single particle, located at the origin. (If all of the particles disappear at some time $t'$, the trial is trapped in the vacuum state for all later times.) A trial consists of sequence $S$ of events, each involving the annihilation or (attempted) creation of a particle. With the help of diagrams reminiscent of the ''percolation substructure'' invoked in defining the CP [10,11], we can write down the probability of sequence $S$; examples are shown in Fig. 1. Each annihilation event carries a factor of $(1-p)/N_p$, each creation event (successful or not) a factor $p/(2dN_p)$. The probability $P_p(S)$ of a sequence $S$, extending to time $t$, is simply the product of all factors associated with events occurring at times $t' \leq t$. Now, for finite $t$, the set $\mathcal{S}_t$ of

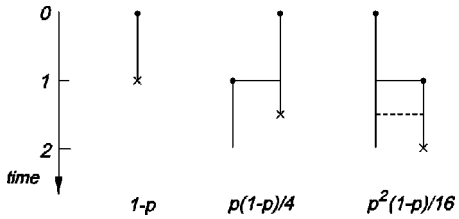


FIG. 1. Examples of event sequences in the one-dimensional contact process starting from a single particle. Vertical lines represent particles, whose birth is marked by a dot, and annihilation by ×. Solid and dashed horizontal lines represent, respectively, successful and unsuccessful creation events. Probabilites are listed beneath each sequence.

*On leave from Department of Physics and Astronomy, Herbert H. Lehman College, City University of New York, Bronx, NY 10468-1589. Electronic address: dickman@fisica.ufmg.br

 

possible sequences is finite, and if $A(S;t)$ is any property of the system (e.g., the number of particles at time $t$), then its expectation is

$$\langle A_t \rangle_p = \sum_{S \in \mathcal{S}_t} P_p(S) A(S;t). \tag{1}$$

In a Monte Carlo simulation we generate a sample $S_1, \ldots, S_N$, drawn from the distribution $P_p(S)$, which yields the estimate $\overline{A}_{t;p} \equiv N^{-1} \Sigma_{k=1}^{N} A(S_k;t)$. From our analysis of $P_p(S)$, it is evident that its $p$-dependence only involves the numbers $c(S)$ and $a(S)$ of creation and annihilation events, respectively; the ratio of the probabilities associated with two different values of $p$ is

$$\omega(S) \equiv \frac{P_{p'}(S)}{P_p(S)} = \left( \frac{p'}{p} \right)^{c(S)} \left( \frac{1-p'}{1-p} \right)^{a(S)}. \tag{2}$$

Thus the reweighted estimate, $\overline{A}_{t;p'} \equiv N^{-1} \Sigma_{k=1}^{N} \omega(S_k) A(S_k;t)$, has expectation

$$\sum_{S \in \mathcal{S}_t} P_p(S) \omega(S) A(S;t) = \langle A_t \rangle_{p'}, \tag{3}$$

and is an unbiased estimator of $A$ in the process with creation probability $p'$.

As in other applications of reweighting, it is not enough to have an unbiased estimator; one must also ensure that the sample generated with creation probability $p$ has a reasonable degree of overlap with a typical sample at $p'$. We expect that as the duration $t_m$ increases, the range of $\lambda$ values for which a sample is useful will narrow. To estimate this range of values, consider a sequence of $r$ events. The probability that exactly $c$ of these are creation attempts is given by the binomial distribution,

$$P(c;r) = \frac{r!}{c!(r-c)!} \frac{\lambda^c}{(1+\lambda)^r}, \tag{4}$$

so that $\langle c \rangle = rp$ and the standard deviation $\sigma$ is given by $\sigma^2 = r\lambda/(1+\lambda)^2$. In a typical sequence generated with creation probability p, the actual number of creation events will be in the range $rp \pm \sigma$, corresponding to a creation rate of $\lambda' \simeq \lambda[1 \pm (1+\lambda)(\lambda r)^{-1/2}]$. Thus the typical fluctuation in $\lambda$ is $\delta\lambda = (1+\lambda)\sqrt{\lambda/r}$. In the two-dimensional CP, for example, one finds that $r \sim 0.7\, t^{1.68}$ for $\lambda \approx \lambda_c \simeq 1.6488$. This corresponds to $\delta\lambda = 0.013$ for $t_m = 1000$. Although the range may appear narrow, it is more than sufficient for ''time-dependent'' simulations, which typically focus on a small interval near $\lambda_c$.

I have applied reweighting to the CP in two and three dimensions, in studies using two kinds of initial states. In the case described above, one studies the survival and spread of activity from a single ''seed'' particle. (The system size must be sufficient to guarantee that particles never reach the boundaries.) The principal quantities of interest are the survival probability $P(t)$, the mean number of particles $n(t)$, and the mean-square distance $R^2$ of particles from the origin. At the critical point these are known to follow asymptotic power laws [12], $P(t) \sim t^{-\delta}$, $n(t) \sim t^{\eta}$, and $R^2(t) \sim t^{z}$. Away from $\lambda_c$ these quantities show deviations from power laws. Since the CP exhibits corrections to scaling of the form $P(t) \sim t^{-\delta}[1 + at^{-\alpha} + \cdots]$ (similarly for $n$ and $R^2$), it is useful to plot derivatives (local slopes of the log-log plots) versus $t^{-1}$ when extracting the critical exponents $\delta$, $\eta$ and $z$ [12]. These exponents are connected by the hyperscaling relation: $4\delta + 2\eta = dz$.

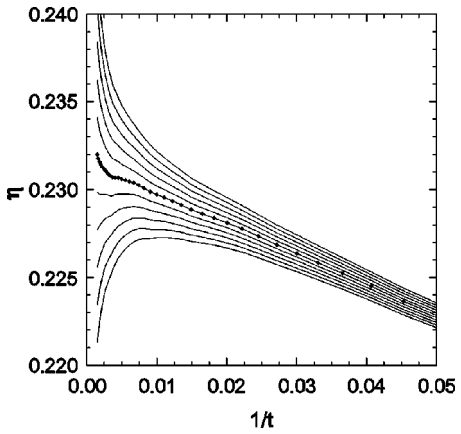


FIG. 2. Local slope plot for exponent $\eta$ in the two-dimensional CP. The middle curve (with data points) marks $\lambda_0 = 1.648\,80$. Curves above and below are for $\lambda$ values at intervals of $\Delta\lambda = 4 \times 10^{-5}$ above and below $\lambda_0$.

The second kind of study begins with all sites occupied, and follows the decay of the particle density $\rho(t)$. In this case the signature of the critical point is power-law decay, $\rho \sim t^{-\theta}$ in the short-time regime, i.e., before the correlation length has attained the system size $L$. A scaling argument implies $\theta = \delta$ [13,14].

As a preliminary test, I compared two results for the survival probability $P(t)$ in the two-dimensional CP at $\lambda = 1.665$, one obtained by reweighting a sample of $N = 10^5$ trials generated at $\lambda = 1.650$, the other from a similar run but without reweighting ($\lambda = 1.665$). The relative difference between the two results for $P(t)$ remains $\leqslant 0.017$ for $t \leqslant t_m = 400$. Since each result has a relative uncertainty of $\sqrt{[1-P(t)]/NP(t)} \simeq 0.01$ for $t = t_m$, $[P(t_m) \simeq 0.085]$, the difference between the two results is fully consistent with sample-to-sample fluctuations.

In two dimensions I performed spreading simulations extending to $t_m = 2980$, on lattices of up to $1200 \times 1200$ sites. Samples generated at a central value, $\lambda_0$, were reweighted so as to study ten additional values, $\lambda = \lambda_0 \pm m\Delta\lambda$, with $m = 1, \ldots, 5$. The general strategy is to use relatively small samples and run times initially, to bracket $\lambda_c$, and then extend the sample size and run time to make finer distinctions. Thus a sample of $10^6$ trials with $t_m = 665$ and $\Delta\lambda = 10^{-4}$ is already sufficient to restrict $\lambda_c$ to the interval [1.648 75,

TABLE I. Critical exponents for DP in two dimensions.

| Exponent | Ref. [2] | Ref. [15] | Present work |
|---|---|---|---|
| $\delta$ | 0.451(3) | 0.4505(10) | 0.4523(10) |
| $\eta$ | 0.229(3) | 0.2295(10) | 0.2293(4) |
| $z$ | 1.133(2) | 1.1325(10) | 1.1316(4) |
| $4\delta + 2\eta - 2z$ | $-0.004(22)$ | $-0.004(8)$ | 0.005(6) |

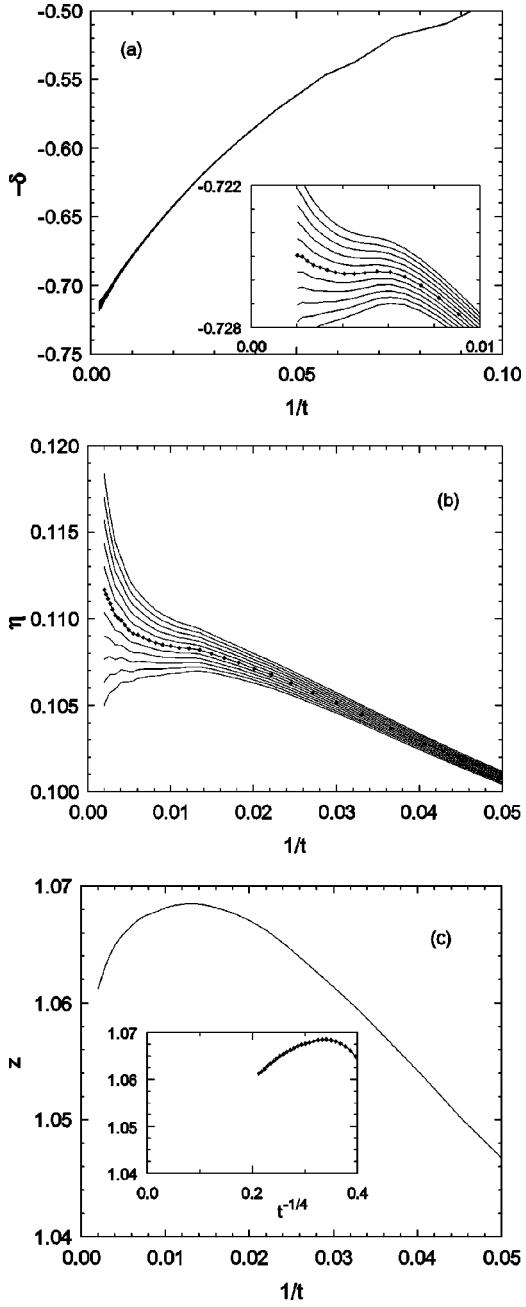


FIG. 3. (a) Local slope plot for exponent $\delta$ in the three-dimensional CP. Inset: detail of $\delta - 4.96t^{-1}$. The middle curve (with data points) marks $\lambda_0 = 1.316\,89$; curves above and below are for $\lambda$ values at intervals of $\Delta\lambda = 2\times10^{-5}$. (b) Local slope plot for exponent $\eta$ in the three dimensional CP. Symbols are as in (a). (c) Local slope plot for exponent $z$ in the three-dimensional CP. The inset shows the same data plotted versus $t^{-1/4}$.

1.648 95]. The most sensitive indicator of criticality is the local-slope plot of $\eta_t$, defined as the derivative of $\ln n$ with respect to $\ln t$. [Numerically $\eta_t$ is estimated from a least-squares linear fit to the $\ln n$ data for a set of $n_i = 17$–$25$ equally spaced values (an increment of 0.1) of $\ln t$; it is plotted versus $t_a^{-1}$, $t_a$ being the geometric mean of the $t$-values over the $n_i$ intervals. $\delta_t$ and $z_t$ are obtained similarly.]

To refine the estimate for $\lambda_c$ I generated two samples of $2.5\times10^7$ trials each, with $t_m = 2980$, $\lambda_0 = 1.648\,80$, and $\Delta\lambda = 4\times10^{-5}$. The critical point was determined from the plot

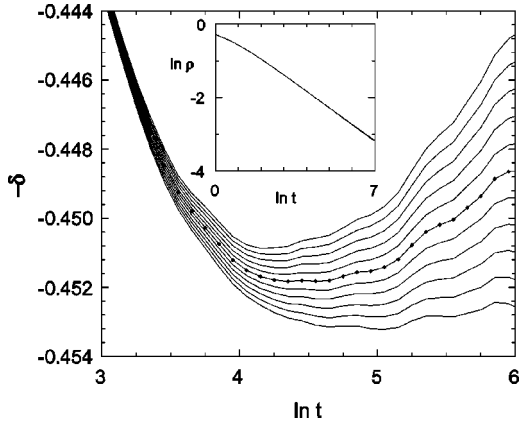


FIG. 4. Local slope plot for exponent $\delta$ in the two-dimensional CP starting with all sites occupied, $L = 128$. The data points mark $\lambda_0 = 1.6490, \Delta\lambda = 5\times10^{-5}$. Inset: decay of the density $\rho$.

of $\eta_t$, which shows a clear deviation from smooth behavior for off-critical values. (Figure 2 shows the $\eta_t$ plot for one of the two runs. Note that the leading correction to scaling does not follow a simple $1/t$ decay, as was also noted for DP in $2+1$ dimensions [2].) These studies yield $\lambda_c = 1.648\,77(3)$, the number in parentheses denoting the uncertainty in the last figure. Extrapolating the local-slope plots, I obtain $\delta = 0.4523(10)$, $\eta = 0.2293(4)$, and $z = 1.1316(4)$, which are in good agreement with, and generally sharper than, the results of previous large-scale simulations of directed percolation [2], and of the ZGB surface catalysis model [15] (see Table I).

Grassberger and Zhang [2] noted that the derivatives of $\ln n(t)$ and $\ln P(t)$ with respect to $\lambda$ (evaluated at $\lambda_c$), grow $\sim t^{1/\nu_{||}}$. Analyzing $n(t)$ in this fashion yields $\nu_{||} = 1.292(4)$, in good agreement with their estimate of 1.295(6).

In three dimensions, I performed four runs of $10^7$ trials each, extending to $t_m = 2208$. (To avoid finite-size effects, I do not use an occupancy array in the three dimensional simulations, but simply search the particle list to detect overlaps.) Two studies used $\lambda_0 = 1.316\,86$, $\Delta\lambda = 3\times10^{-5}$; in the others, $\lambda_0 = 1.316\,89$ and $\Delta\lambda = 2\times10^{-5}$. Figure 3 shows the local slopes for one of the latter runs. While the extrapolation of $\eta$ is straightforward, the strong linear correction to $\delta$ ($\delta_t \simeq \delta - 4.96t^{-1} + \cdots$), renders it advantageous to subtract the linear term when estimating the exponent [inset of Fig. 3(b)]. In the case of $z$, the curves for all $\lambda$ values are virtually identical. It is difficult to extrapolate the $1/t$ plot; the present estimate is derived by extrapolating the local slope plotted versus $t^{-1/4}$, as in Fig. 3(c). Averaging over the results for the four runs yields the following estimates for the three-dimensional CP:

$$\lambda_c = 1.316\,86(1), \quad \eta = 0.110(1),$$

$$\delta = 0.7263(11), \quad z = 1.042(2)$$

(the uncertainties represent one standard deviation). These are in good accord with hyperscaling: $4\delta + 2\eta - 3z = -0.001(12)$. The present results are compatible with Jensen's estimates of $\lambda_c = 1.3168(1)$, $\eta = 0.114(4)$, and $\delta$

$=0.730(4)$, but not with his value $z=1.052(3)$ [16]. Analysis of $d\ln n(t)/d\lambda$ yields $\nu_{||}=1.114(4)$, just consistent with Jensen's result, 1.105(5).

I studied the initial decay of the density (starting with all sites occupied), in the two-dimensional CP for system sizes $L=32$, 64, and 128. Figure 4 shows the results of one of three sets with $L=128$, $10^5$ trials, $\lambda_0=1.6490$, and $\Delta\lambda=10^{-4}$. (The studies for $L=32$ and 64 used similar parameters, in runs of $5\times10^5$ and $2\times10^5$ trials, respectively.) For the relatively short runs employed here ($t_m\leqslant1096$), all trials survive up to $t_m$. While the $\rho(t)$ curves (inset) for different $\lambda$ values are indistinguishable, the local slopes (main graph) vary quite systematically with $\lambda$. Since the power law $\rho\sim t^{-\delta}$ obtains for finite times not $t\to\infty$, I plot the local slope versus $\ln t$ in this case. One can distinguish three regimes: an initial phase in which $\delta_t$ increases for all $\lambda$ values, a late stage in which it decreases, as $\rho(t)$ approaches a value $\sim L^{-\beta/\nu_\perp}$ as predicted by finite size scaling, and an intermediate regime in which $\delta_t$ is more or less constant. Associating $\lambda_c$ with the $\delta_t$ most nearly constant in the intermediate regime yields $\lambda_c=1.6492(1)$ for $L=32$, 1.6491(1) for $L=64$, and 1.648 98(5) for $L=128$. The corresponding estimates for $\delta$ (from the flat portion of each curve) are 0.4508(10) for $L=32$ and 0.4520(5) for $L=64$ and 128. Thus the $\lambda_c$ estimates appear to be approaching the value derived from spreading simulations; the two kinds of studies yield consistent results for $\delta$.

In summary, I propose a simple reweighting scheme for nonequilibrium lattice models, and apply it to the contact process in two and three dimensions. Since spreading simulations are usually repeated for five or so different $\lambda$ values, reweighting yields roughly an order-of-magnitude speedup. In addition to improving efficiency, using the same sample to study all parameter values eliminates the effects of independent fluctuations, which complicate determination of $\lambda_c$ and the critical exponents. These computational advantages have permitted determination of the critical parameters of the three-dimensional CP to unprecedented precision. One may expect reweighting to find wide application in simulations of nonequilibrium critical phenomena, including models with multiparticle processes.

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