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ESTIMATING THE CRITICAL VALUES OF STOCHASTIC GROWTH MODELS

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Abstract

Interacting particle systems provide an attractive framework for modelling the growth and spread of biological populations and diseases. One problem with their use in applications is that in most cases the existing information about their critical values and equilibrium densities is too crude to be useful. In this paper we describe a method for estimating these quantities that does not require very much computer time and produces fairly accurate results.

CONTACT PROCESS; CRITICAL VALUES

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In this paper we describe a method for estimating the critical values of interacting particle systems and apply the method to two special cases of two examples. In each of the systems we consider the state of the process at time t is $\xi_t \subset \mathbb{Z}^d$ and we think of the $x \in \xi_t$ as being occupied by a 'particle'. In the definitions below, $\mathcal{N}$ is the set of neighbors of 0. For example, $\mathcal{N} = \{y : \| y \|_1 = 1\}$, the $2d$ nearest neighbors.

Example 1. The threshold contact process.

(a) Occupied sites become vacant at rate 1.

(b) A vacant site x becomes occupied at rate β if at least one of its neighbors $y \in x + \mathcal{N}$ is occupied.

Example 2. The basic contact process.

(a) Occupied sites become vacant at rate 1.

(b) An occupied site gives birth to a new particle at rate β. A particle born at x is sent to a randomly chosen neighbor $y \in x + \mathcal{N}$. If y is occupied then no birth occurs.

To describe the questions we want to answer we have to introduce some 'well known' results about these processes. More detail can be found in Liggett (1985) or Durrett (1988). The two systems described above are *attractive*, i.e. if $\xi_0 \subset \xi'_0$ then we can define realizations of the process starting from these initial configurations on the same space

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in such a way that $\xi_t \subset \xi_t'$ for all $t \geqq 0$. An immediate consequence of this property is that if we start from $\xi_0^1 = \mathbb{Z}^d$ then as $t \to \infty$, $\xi_t^1 \Rightarrow \xi_\infty^1$ where $\Rightarrow$ denotes weak convergence, which in this setting is just convergence of finite-dimensional distributions. General results imply that ξ_∞^1 is the largest possible stationary distribution for the system. Of course it may be the trivial stationary distribution $\delta_\varnothing$, the point mass on the $\varnothing$, and in this case we say that the system *dies out*. We define the *critical value* in general by

$$\beta_c = \inf\{\beta : \xi_\infty^1 \neq \delta_\varnothing\}$$

and write $\beta_c(i)$ for the critical value of Example i when $d = 2$ and $\mathcal{N} = \{y : \| y \|_1 = 1\}$.

To get lower bounds on $\beta_c(i)$, we observe that the birth rate per particle is at most 4β in Example 1 and at most β in Example 2. Using the equation for $d\boldsymbol{P}(0 \in \xi_t^1)/dt$ it is easy to see that

$$(1) \qquad \beta_c(1) \geqq 1/4, \qquad \beta_c(2) \geqq 1.$$

Upper bounds on the critical values are more difficult, but Liggett (1991) (see Cox and Durrett (1991) for a proof of this corollary of his result) and Holley and Liggett (1978) have shown

$$(2) \qquad \beta_c(1) \leqq 1.14, \qquad \beta_c(2) \leqq 4.$$

The bounds in (1) and (2) are not very tight but are the best known results and are much better than what is known about many other examples. This brings us to our main question: how do you estimate β_c from computer simulation? The first and simplest answer is to run the system and see what happens. Consider Example 2 on a 200×200 lattice with *periodic boundary conditions*, i.e. points x and y are neighbors if there is a $z \in \mathcal{N}$ so that for $i = 1, 2$, $x_i - y_i = z_i \bmod 200$. If we take $\beta = 1.45$ and run the process until time 200 then the system dies out. If we take $\beta = 1.85$ and plot the fraction of occupied sites at times $t \in [0, 200]$ we get a curve (see Figure 1) that suggests that the system is converging exponentially rapidly to an equilibrium in which about 28% of the sites are occupied.

The last experiment gives us a crude estimate of $\beta_c(i)$. With a little more thought we can extract quite a bit more information from one simulation. Our first step is to change the time scale so that:

(a) Occupied sites become vacant at rate δ.

(b) An occupied site gives birth to a new particle at rate 1. A particle born at x is sent to a randomly chosen neighbor y. If y is occupied then no birth occurs.

Our second step is to define a process $\zeta_t : \mathbb{Z}^2 \to [0, 1]$ so that for all $\delta \in [0, 1]$

(3) $\qquad \xi_t^\delta(x) \equiv 1_{(\zeta_t(x) \geq \delta)}$ is a realization of the process with death rate δ.

In words, $\zeta_t(x)$ is the largest value of $\delta \leqq 1$ for which site x is occupied at time t. To construct $\zeta_t(x)$ we define for each site two rate-1 Poisson processes $\{S_n^x, n \geqq 1\}$ and $\{T_n^x, n \geqq 1\}$, a sequence of random variables $\{U_n^x, n \geqq 1\}$ that are uniform on (0, 1), and

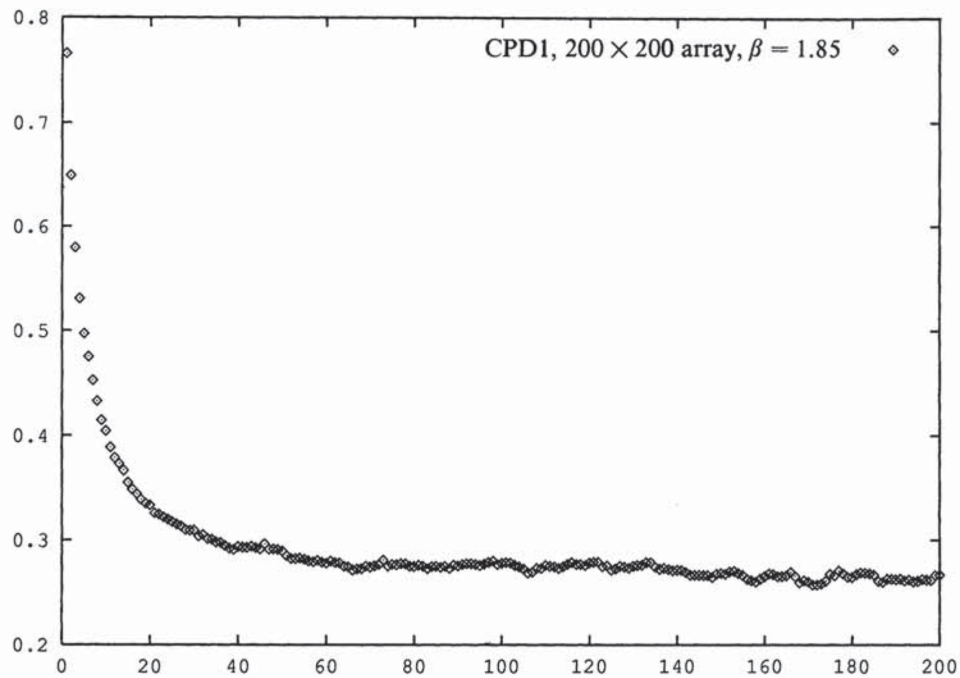

Figure 1

a sequence of random variables $\{Y_n^x, n \geqq 1\}$ that are uniform on $x + \mathcal{N}$. All these sequences are supposed to be independent. The evolution is then computed using the following rules:

(a) at times $s = S_n^x$ we set $\zeta_s(x) = \zeta_s(Y_n^x)$ if $\zeta_s(x) < \zeta_s(Y_n^x)$,

(b) at times $t = T_n^x$ we set $\zeta_t(x) = U_n^x$ if $\zeta_t(x) > U_n^x$.

To see that the transitions go in the right direction in (a) and (b) note that increasing the value at x makes that site occupied in more processes, while decreasing the value makes it vacant more. Using the fact that the set of T_n^x with $U_n^x < \delta$ is a Poisson process with rate δ it is easy to check that (3) holds.

The last construction is convenient for mathematicians but not for a computer. To simulate $\zeta_t(x)$ on $\Lambda = \{0, 1, \cdots, L-1\}^2$ with periodic boundary conditions we use the following algorithm:

(a) pick a site x at random,

(b) flip a fair coin to see if the event should be a birth or death,

(c) if the event is a death we generate an independent U that is uniform on (0, 1) and set $\zeta(x) = U$ if (and only if) $U < \zeta(x)$,

(d) if the event is a birth we pick a neighbor y at random and set $\zeta(x) = \zeta(y)$ if (and only if) $\zeta(y) > \zeta(x)$.

The sequence of ζ's generated by the last procedure corresponds to the embedded jump chain for ζ_t (on $\Lambda = \{0, 1, \cdots, L-1\}^2$ with periodic boundary conditions). To see this note that the Markov property of the Poisson process implies that the site and type of the nth arrival are i.i.d. and uniformly distributed over the set of possibilities. In passing from the mathematical to the computer definition of the process we ignore the amount of time that the process spends in each state, but this is harmless. The asymptotic fraction of time a site is occupied is the same in both processes.

Since the algorithm just described simulates the process simultaneously for all values of $\delta \in [0, 1]$ we can estimate the limiting density $\rho(\delta) = \boldsymbol{P}(0 \in \xi^1_\infty)$ in the obvious way. Start with $\zeta_0(x) \equiv 1$. This corresponds to having all sites occupied for all $\delta \leqq 1$. Run the process on $\{0, 1, \cdots, L-1\}^2$ out to time T, (that is, we perform L^2T transitions) and let $\hat{\rho}(\delta)$ be the fraction of sites with $\zeta(x) \geqq \delta$. Figure 2 shows the curve that results when $L = 200$ and $T = 1000$. As the reader can probably guess from the smoothness of the graph, the curve that results is not very random.

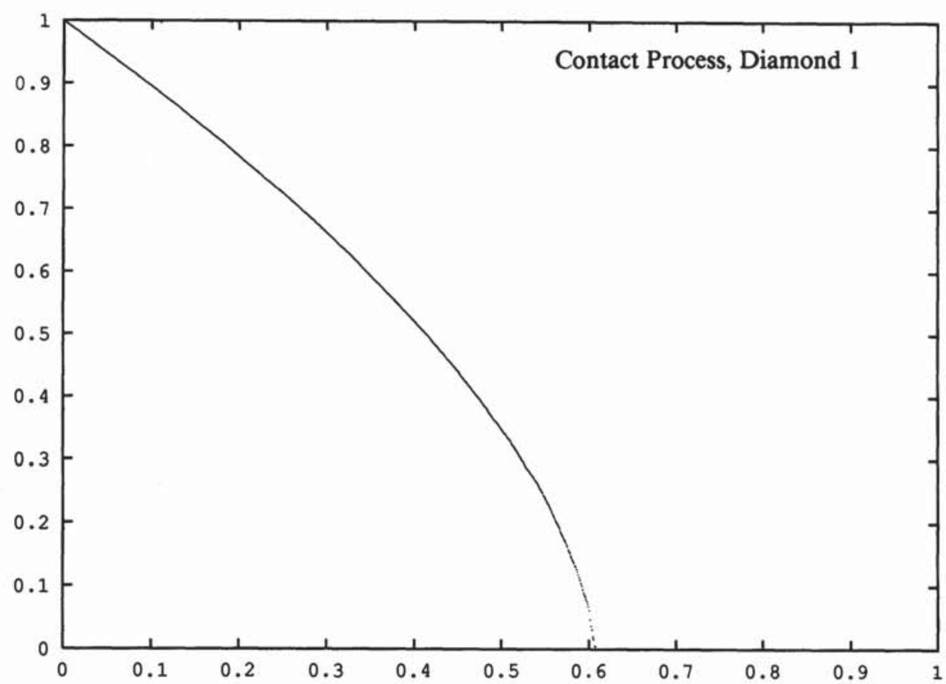

Figure 2

The curve in Figure 2 suggests that $\delta_c \equiv 1/\beta_c$ lies in (0.6, 0.62). To get more accurate results we will use a method that is common in the physics literature (see e.g. Dickman and Burschka (1988) pp. 133–134). We pick a sequence of values δ_i, compute our estimates $y_i = \hat{\rho}(\delta_i)$, use linear regression to fit

$$\log y_i = a + b \log(\gamma - \delta_i) \tag{4}$$

for various values of γ, and then use the γ that minimizes the sum of the squared errors as our estimate of δ_c. This recipe is based on the assumption that the limiting density satisfies

$$\rho(\delta) \sim C(\delta_c - \delta)^b \qquad \text{as } \delta \uparrow \delta_c \tag{5}$$

TABLE 1
Simulation data and estimates for the basic contact process in $d = 2$ with $\mathcal{N} = \{y : \| y \|_1 = 1\}$

0.565	0.570	0.575	0.580	0.585	0.590	0.595	0.600
0.201756	0.187177	0.171103	0.154968	0.136846	0.118090	0.095542	0.066958
0.202806	0.187920	0.172399	0.154910	0.137894	0.119404	0.096929	0.071865
0.204008	0.189009	0.173444	0.157070	0.139735	0.119517	0.098390	0.070650
0.203487	0.188987	0.173302	0.157512	0.138902	0.117495	0.097007	0.069811
0.202691	0.187921	0.172019	0.155705	0.137787	0.118466	0.096439	0.067464

$\delta_c = 0.6058$	$b = 0.5638$	sse = 0.000084
$\delta_c = 0.6078$	$b = 0.6094$	sse = 0.000070
$\delta_c = 0.6066$	$b = 0.5740$	sse = 0.000080
$\delta_c = 0.6070$	$b = 0.5962$	sse = 0.000195
$\delta_c = 0.6058$	$b = 0.5614$	sse = 0.000098

where $f(x) \sim g(x)$ means $f(x)/g(x) \to 1$ as $x \to 0$. The asymptotic behavior in (5) is believed to hold in a wide variety of models (see for instance Janssen (1981) or Grassberger (1982)). The exponent b is a critical exponent usually denoted by β in the physics literature. Since β is our birth rate we prefer the non-traditional designation here.

The data in Table 1 show what happened in five applications of this technique to Example 2. To estimate the density we ran the system with $L = 200$ and from times 3000–10 000 we examined the density of occupied sites every 10 units of time for the indicated parameter values, averaging the 700 observations to get the number in the table. The reader should note that we waited until time 3000 to allow the density to converge to equilibrium (this time was picked by examining the behavior of the density versus time in earlier runs), and that we did not take values of δ too close to the critical value because there the estimated values have large fluctuations. Table 1 gives the values of δ_c and b that were obtained. As the reader can see, the estimates of δ_c do not fluctuate very much but the values of b we compute vary considerably. The values we obtained are consistent with the estimates one can find in the physics literature. Brower et al. (1978) give $\delta_c \approx 0.607$ (our δ_c is their $T_c/4$) and with the help of definitions in Cardy and Sugar (1980) one can compute that $b \approx 0.585$. The results just quoted are for 'Reggeon field theory', a physical system that is equivalent to the basic contact process, see Grassberger and de la Torre (1979). To break some new ground we tried our method on the basic contact process in $d = 2$ with $\mathcal{N} = \{y : \| y \|_\infty = 1\}$. Table 2 gives the data and the estimates that were obtained.

The method described above for the basic contact process, after a simple modification, can be applied to the threshold contact process on $d = 2$ with $\mathcal{N} = \{y : \| y \|_1 = 1\}$. The first step is to construct a simulation of the process on $\Lambda = \{0, 1, \cdots, L-1\}^2$ for all values of $\beta \in (0, 1)$. We restrict our attention to this range of β's since we expect $\beta_c < 1$. We skip the formulation of the process in continuous time and go directly to the computer implementation. The rules are similar to those of the contact process, but the roles of births and deaths are interchanged since we are now thinking of $\zeta(x)$ as being the smallest value of β for which the site is occupied:

(a) pick a site x at random,

TABLE 2
Simulation data and estimates for the basic contact process in $d = 2$ with $\mathcal{N} = \{y : \|y\|_\infty = 1\}$

0.640	0.645	0.650	0.660	0.665	0.670	0.675	0.680	0.685	0.690
0.197356	0.186144	0.174303	0.149870	0.136977	0.122005	0.105020	0.087854	0.067079	0.039907
0.198550	0.186745	0.174749	0.149549	0.136050	0.121693	0.106166	0.089208	0.070799	0.048279
0.198122	0.186976	0.175197	0.149662	0.135723	0.121786	0.106173	0.087697	0.067154	0.044513
0.199175	0.188028	0.176177	0.151025	0.137936	0.123157	0.106734	0.090322	0.071316	0.045715
0.198609	0.187124	0.175380	0.150437	0.136795	0.122231	0.106565	0.087491	0.065672	0.039821

$\delta_c = 0.6935$	$b = 0.5883$	sse $= 0.000086$
$\delta_c = 0.6962$	$b = 0.6400$	sse $= 0.000018$
$\delta_c = 0.6952$	$b = 0.6336$	sse $= 0.000376$
$\delta_c = 0.6948$	$b = 0.6010$	sse $= 0.000233$
$\delta_c = 0.6937$	$b = 0.6015$	sse $= 0.000325$

(b) flip a fair coin to see if the event should be a birth or death,

(c) if the event is a death we set $\zeta(x) = 2$ to indicate that the site is vacant for all values of $\beta \in (0, 1)$,

(d) if the event is a birth we generate an independent U that is uniform on $(0, 1)$, let μ be the minimum value of $\zeta(y)$ at the neighbors of x and set $\zeta(x) = \mu \vee U$ if (and only if) $\zeta(x) > \mu \vee U$.

The explanation for the algorithm just described is similar to the one for the basic contact process. To check (d), we note that the arrival in the birth Poisson process will result in an attempted birth if and only if $\beta < U$ and there is an occupied neighbor if and only if $\beta < \mu$.

TABLE 3
Simulation data and estimates for the threshold contact process in $d = 2$ with $\mathcal{N} = \{y : \|y\|_1 = 1\}$

0.520	0.515	0.510	0.505	0.500	0.495	0.490	0.485	0.480	0.475
0.156908	0.147908	0.138387	0.127824	0.116877	0.104858	0.091512	0.074972	0.057401	0.031316
0.157799	0.149075	0.139558	0.129311	0.118361	0.106314	0.092922	0.077515	0.059076	0.035973
0.158014	0.149019	0.139224	0.129132	0.118086	0.106558	0.092419	0.076550	0.058795	0.034451
0.157529	0.148579	0.139130	0.129097	0.117853	0.105908	0.092067	0.076985	0.057221	0.026437
0.156985	0.147983	0.138522	0.128505	0.117261	0.105718	0.092249	0.077888	0.058389	0.030872

$\beta_c = 0.4725$	$b = 0.5476$	sse $= 0.000159$
$\beta_c = 0.4716$	$b = 0.5581$	sse $= 0.000205$
$\beta_c = 0.4719$	$b = 0.5543$	sse $= 0.000168$
$\beta_c = 0.4736$	$b = 0.5126$	sse $= 0.000031$
$\beta_c = 0.4729$	$b = 0.5194$	sse $= 0.000086$

Once we know how to simulate the threshold contact process, its critical value can be estimated as before. Table 3 gives the data and the estimates that we obtained. The five estimates of δ_c suggest strongly that $\delta_c < 0.5 < 1$. We are interested in the conclusion $\delta_c < 1$ because the survival of the threshold contact process with $\delta = 1$ implies that coexistence occurs in the threshold voter model that uses the same set of neighbors. See the discussion after Theorem 4 in Cox and Durrett (1991). It is conjectured that

TABLE 4
Simulation data and estimates for the threshold contact process in $d = 1$ with $\mathcal{N} = \{-2, -1, 1, 2\}$

0.90	0.89	0.88	0.87	0.86	0.85	0.84	0.83	0.82
0.347724	0.336823	0.324793	0.311667	0.296228	0.278344	0.256045	0.227495	0.184683
0.347846	0.336897	0.324812	0.311581	0.295896	0.277866	0.256227	0.228511	0.186545
0.347393	0.336585	0.324597	0.311030	0.295543	0.277243	0.254816	0.226734	0.184835
0.348652	0.337927	0.326005	0.312772	0.297339	0.279550	0.258626	0.230826	0.189139
0.347920	0.337078	0.324876	0.311679	0.296152	0.278399	0.256484	0.228065	0.189437

$\beta_c = 0.8115$	$b = 0.2704$	sse = 0.000011
$\beta_c = 0.8109$	$b = 0.2731$	sse = 0.000003
$\beta_c = 0.8109$	$b = 0.2772$	sse = 0.000014
$\beta_c = 0.8109$	$b = 0.2675$	sse = 0.000002
$\beta_c = 0.8100$	$b = 0.2782$	sse = 0.000039

coexistence occurs in the threshold voter model in $d = 1$ when $\mathcal{N} = \{-2, -1, 1, 2\}$. To support this conjecture we have investigated the critical value of the corresponding threshold contact process. The results reported in Table 4 suggest $\delta_c < 0.82 < 1$.

The conclusion we would like the reader to draw from the four examples is the following: given a one-parameter family of stochastic growth models (translation-invariant finite-range processes $\xi_t \subset \mathbb{Z}^d$ with $\varnothing$ an absorbing state) one can estimate the critical value for the existence of a non-trivial stationary distribution by estimating the equilibrium densities at 8–10 values and then fitting a straight line as in (4). In many situations one can simulate the process simultaneously for all parameters in the range of interest so the estimation can be done from one run.

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