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A method for finding bounds on critical values for non-attractive interacting particle systems

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Abstract. The method is to use a computer to find a function for the process that always has negative expectation by considering all relevant configurations of 0's and 1's at the boundary of a finite process in one dimension. It is shown that a branching annihilating random walk will die out if the diffusion parameter ρ is greater than 0.176. The method may also be applied to attractive processes, and is used for the contact process in one dimension obtaining the same values as Ziezold and Grillenberger (1988) for up to 10 places in from the boundaries.

1. Introduction

This paper is concerned with the spread of finite sets of particles situated on a lattice. Specifically we shall suppose that each position on the lattice of integers, $\mathbb{Z}$, is either occupied (1) or unoccupied (0) so that the state space is $\{0, 1\}^{\mathbb{Z}}$. (Occupied and unoccupied can also be thought of as spin-up and spin-down.) Particles interact with their neighbours so that the set of occupied sites of the lattice evolves in time. The rates at which these interactions occur will be the parameters of the process. Certain types of processes exhibit critical behaviour, that is, for some values of the parameters, finite sets of particles tend to grow and for other values they die out almost surely (a.s.). The purpose of this paper is to present a method of getting bounds on the critical values of the parameters.

The contact process has been one of the most widely studied of all interacting particle systems. Particles die at rate 1, so that independently of all other sites a 1 may flip to a 0, or particles may spread at rate b (often λ), so that any pair of adjacent sites of the form 01 may flip to 11 independently of all other possible interactions. It can be considered as a model of an infection, with dying equivalent to recovery from the disease. These systems have a critical behaviour that is like that in thermal equilibrium although they start far from equilibrium. Substantial work has been done finding bounds on the critical value at which a phase transition occurs. The work is summarized in Konno (1994), ch 3. The best lower bound for b given there is 1.539 (Ziezold and Grillenberger 1988), and the best upper bound 1.942 (from Liggett 1994).

The technique given in this paper is to produce a function that gives a 'score' to each finite configuration. As the process evolves, depending on the parameters, this score will either tend to decrease or increase, and this will correspond to the process dying out or spreading to ∞. (These scores will be used to define a supermartingale for the process where possible. Scores may also be thought of as Lyapunov functions.)

The scores will have three components, the distance from the leftmost to the rightmost particle plus subsidiary scores given to their m-configurations, that is the 2^m possible sets of

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sites m places in from those end particles (m to be chosen). In the contact process, if the m sites next to an end particle are all occupied, it will be easier for the process to spread than if they are unoccupied. The score when the m places are occupied will be greater than that when they are not. This is because the contact process is an 'attractive' interacting particle system (IPS), that is, the more particles, the more likely the process is to spread. However, when the IPS is not attractive because a particle may be annihilated by a neighbour, it is not at all clear which is the most advantageous m-configuration. How to find it is part of the purpose of this paper, and once it is found, a bound on the critical values of the parameters follows.

The branching annihilating random walk (BARW) was introduced by Bramson and Gray (1985) after hearing a talk given by S Ulam. They imagined that each particle independently performed a random walk on the integer lattice $\mathbb{Z}$ at rate ρ and also placed offspring on a neighbouring site at rate 1. When a particle landed on a site already occupied, the two particles annihilated each other. They showed that for sufficiently small ρ the BARW could survive and that for sufficiently large ρ, it would die out. This paper demonstrates that when $\rho > 0.176$ the process will die. This value is obtained by looking at the configurations eight places in from the outer 1's of a finite configuration. The bound derived by simply looking 1 place in from the end is $1/3$, and by increasing the number of places from 1 to 8, the value is lowered and approaches the value of 0.103 obtained by Inui (1993) by simulation. It should be noted that it has not been proved that a critical value of ρ exists for the BARW although it would seem reasonable that it should do.

In this paper the BARW is only considered on $\mathbb{Z}$, and we speed it up by rate 2. In the notation of Sudbury (1997b) the BARW is defined by the possible interactions between pairs of neighbouring sites: birth (a particle adds a particle to an empty neighbouring site, $10 \to 11$) at rate $b = 1$; exclusion (a particle jumps to an empty site, $10 \to 01$) at rate $e = \rho$; annihilation (either one of two neighbouring particles jumps onto the other and they annihilate, $11 \to 00$) at rate $a = 2\rho$; and coalescence (one particle places an offspring on an occupied neighbouring site annihilating the particle there, $11 \to 10$) at rate $c = 1$.

There is one other flip we shall use later: death (a particle with an unoccupied neighbouring site dies, $10 \to 00$) at rate d. (Note, in this paper we do not consider flips from the state 00.)

Because the method is simpler to explain for the contact process, we treat this case before that of the BARW.

2. The contact process in one dimension

We consider a contact process with initial configuration finite. We aim to find bounds on the leftwards spread of the process by looking at the possible changes that can occur to the configuration m places to the right of the leftmost occupied site. There are 2^m possible states which we shall designate by the integers $0, 1, \ldots, 2^m - 1$ for which they are the binary expansions. For example, with $m = 3$, the left-hand end of the form $\ldots 0110110 \ldots$ has m-configuration 101, the binary expansion of 5.

The m-configuration is not a closed system because its evolution depends on the configuration to its right. Since we are seeking lower bounds to the critical value we shall be looking for the configurations to the right which are most advantageous for leftwards spread. We may imagine a kind of Maxwell's demon who sits at the right end of the m-configuration and, when the m-configuration changes, instantaneously adjusts the right configuration.

Let us first see what possible choices of right configuration the demon can make. We shall illustrate this with the case $m = 2$ and state $i = 1$ corresponding to the left-hand situation $\ldots 0101x_1x_2 \ldots .\ x_1, x_2, \ldots$ is the right configuration. At rate b a 1 is put to the left of the leftmost 1 so that the new left end is $\ldots 01101x_1x_2 \ldots .$ The m-configuration jumps to 10 ($i = 2$) and the process spreads by 1. At rate $2b$ a 1 is put between the 1's. This time the m-configuration jumps to 11 ($i = 3$), but the process does not spread. Or the 1 dies at rate 1, in which case the process contracts by 2 and the next m-configuration is x_1x_2. Thus when the m-configuration jumps to the state 1, the demon has four possible choices for the right configuration which it will instantaneously create, and this choice determines the rates at which the m-configuration evolves stochastically. If $j = 2x_1 + x_2$, then the rates out of the state 1 are $q_{12} = b$, $q_{13} = 2b$, $q_{1j} = 1$ where j may of course be 2 or 3, in which case the rate 1 is added to the other rates. Once a demon has decided which right configuration to choose for each state, all the rates q_{ij}, $i, j = 0, 2^m - 1$, are determined and a Markov process with state space the set of m-configurations is defined. Since there are several possibilities for the choice of right configuration for each m-configuration, the overall number of possible Q-matrices and their corresponding Markov processes is large. For the case $m = 2$ it can be shown to be 128. The purpose of this paper is to give a method for finding the particular set of right configurations most favourable for leftwards spread, or to put it another way, the most favourable Q-matrix. (Although this is not needed here, the Q-matrix determines the forward equation for the probabilities and equals $-H$, the negative of the Hamiltonian.)

A particular problem is caused by the state $i = 0$ which, for the case $m = 2$, would mean the left-hand end was $\ldots 0100x_1x_2 \ldots .$ The left-hand 1 dies at rate 1 and when it does so, the left-hand end retreats to the next 1 to the right, but this may be an arbitrarily large number of spaces away. We can put 3 as a lower bound to the number of spaces contracted and this is obviously the most advantageous value. It is because we cannot bound above the size of the contraction that the method presented in this paper only gives one-sided bounds.

If the process is finite and has leftmost and rightmost 1's in positions $-l$ and r, respectively, and the left m-configuration is in state i and the right in state j, then the total score for the process is $L = l + r + S_i + S_j$ where the set of 'scores' $\{S_i\}$ corresponding to states i are to be determined. Given a value of b, if we can find a set of values S_i for which the rate of change of the expectation of L is negative in every state i, then b will be below the critical value for the contact process.

In general in the analysis of IPS, for each state i, we consider all possible relevant right configurations and their associated q_{ij} and determine which combination of right configurations is the 'most advantageous'. However, the contact process is well known to be 'attractive', and so it is not surprising that the correct strategy for the demon is to always make the right configuration 'all 1's'. When the leftmost particle moves k places to the left the change in score is k. Because we are only considering the most advantageous right configurations, when the left-hand 1 dies in the state $i = 0$, we assume the left-hand 1 moves $m + 1$ places to the right contributing $-(m + 1)$ to the change in L.

We write the rate of change of the expected leftmost position when in state i as a_i, then with a set of transition rates q_{ij} determined by a particular set of right configurations, the rate of change of the expected score when in state i is

$$a_i + \sum_{j \neq i} q_{ij}(S_j - S_i).$$

Our general task is to find $\{S_i\}$ s.t. for a given b, these expressions are negative for all possible sets of transition rates q_{ij}, but with the contact process this procedure is much simplified by knowing the most advantageous right configurations already. We put $S_0 = 0$.

Given any particular $2^m \times 2^m$ Q-matrix Q, Sudbury (1997a) defined an associated $2^m - 1 \times 2^m - 1$ matrix Q^* with

$$q^*_{ij} = q_{ij} \qquad i, j \neq 0 \qquad q^*_{ii} = -\sum_{j \neq i} q_{ij}.$$

The required system of inequalities (reversed in Sudbury (1997a)) may be written

$$\sum q_{0j} S_j + a_0 \leqslant 0 \qquad Q^* \underline{S} \leqslant -\underline{a} \tag{1}$$

where $\underline{S} = (S_1, \ldots, S_n)^{\mathrm{T}}$.

The paper showed $(Q^*)^{-1}$ was negative, so that (1) implies $\underline{S} \geqslant -(Q^*)^{-1}\underline{a}$. Since $q_{0j} \geqslant 0$ for all j, the first inequality in (1) will be satisfied most readily by the smallest possible $\underline{S}$. Thus it is sufficient to calculate $\underline{S} = -(Q^*)^{-1}\underline{a}$ and check the sign of $\sum q_{0j} S_j + a_0$. If this is negative, $\underline{S}$ is called the *minimum score* for the particular Q-matrix.

A computer program was therefore written which would calculate the Q-matrix for any given input of pairwise flip rates and given set of right configurations for each state of the IPS. The chief programming difficulties arise when the leftmost 1 moves to the right. If it moves $k \leqslant m$ spaces, then the last $m - k$ places of the previous m-configuration become the first $m - k$, and there are 2^k possible ways in which the new m-configuration can be formed. $k > m$ only occurs in the contact process when $i = 0$ and the leftmost 1 dies. There are then 2^m possible new m-configurations.

As mentioned above, the contact process is an attractive model and thus the search for the most advantageous set of right configurations is simple. Define Q^1 to be the Q-matrix when the $m + 1$ positions to the right of the m-configuration are always 1's. Let Q be any other Q-matrix. Given any two states i, j we write $i \supset j$ if the set of 1's in the binary expansion of i contains the set of 1's in that of j. Then we have the following lemma.

Lemma 1. If the set $\{S_i\}$ has the property that $S_i \geqslant S_j$ when $i \supset j$, then

$$\sum Q^1_{ij}(S_j - S_i) > \sum Q_{ij}(S_j - S_i)$$

where Q is any other possible Q-matrix.

Proof. There are two ways in which the Q-matrices can differ. First, $x_1 \neq 1$ for some state i in the definition of Q. If i has last digit 0, then $x_1 = 1$ gives a contribution of b to the transition from i to $i+1$, and this gives a non-negative contribution to $\sum Q^1_{ij}(S_j - S_i)$ since in that case $i + 1 \supset i$. The other way occurs when the leftmost 1 in i dies and i jumps to a state j which may be partly made up of the rightmost digits of i or may not. In either case, if j is the state i jumps to in the Q-situation and if it is j^1 in the Q^1-situation, then $j^1 \supset j$ and $S_{j^1} \geqslant S_j$. □

The procedure for finding a suitable set $\{S_i\}$ is thus very simple.

(1) Select a value of b.

(2) Calculate the transition matrix Q^1 and associated matrix $(Q^1)^*$.

(3) Solve the equation $\underline{S} = -(Q^*)^{-1}\underline{a}$ with $Q = Q^1$.

(4) Find the sign of $\sum q_{0j} S_j + a_0$.

(5) If the sign is negative, try a larger value of b, if positive, try a smaller value until the changepoint is found.

(6) With the $\{S_i\}$ found for the b just below the changepoint, test $S_i \geqslant S_j$ when $i \supset j$ for all pairs i, j.

If the test is satisfied, then the left-hand contribution to the rate of change of the expectation of L is negative whatever the configuration to the right of the m-configuration. Because of the obvious symmetry with the right-hand contribution, it would then follow that L is a supermartingale. Since it is well known that the contact process must either die out or spread to infinity, it is obvious that the process would then die out.

The procedure was carried out for the cases $m = 2, 3, \ldots, 10$, when it had to be stopped as the VAX computer being used would not handle arrays of size 2048×2048. The S_i at the changepoint values b_m all satisfied the conditions of lemma 1 and thus the b_m are all lower bounds to b_c, the critical value for the one-dimensional contact process.

m	b_m
2	1.279
3	1.342
4	1.387
5	1.420
6	1.445
7	1.465
8	1.481
9	1.495
10	1.506

These numbers are in agreement with those of Ziezold and Grillenberger (1988). Although their method is different, it is in fact equivalent to the method used here. They considered the cases $m = 2, 3, \ldots, 14$ up to 20 decimal places, finally achieving a lower bound of $1.538\,848\ldots$ and so on.

3. The branching annihilating random walk

In this section we introduce the idea that it may be more advantageous to derive bounds on critical values of a process by considering a dual of that process. Duals have been widely used in the theory of IPS and there are extensive discussions in Liggett (1985) and Sudbury and Lloyd (1995). The only part of the theory needed here is that a positive probability of survival for an IPS implies a positive probability of survival for all of its duals.

Sudbury and Lloyd (1995) gave an algebraic formula which allowed the duals of any IPS with pairwise interactions to be written down. This formula was much simplified in Sudbury (1997b). An IPS given by the rates a, b, c, d, e defined in the introduction of this paper is dual with duality parameter x to the IPS with rates given by

$$a' = a + 2xy \qquad b' = b - y \qquad c' = c - (1 + x)y \qquad d' = d - y \qquad e' = e + y$$

where $y = (d - a - c - bx)/(1 - x)$. The primed rates given above only define an IPS when all rates are $\geqslant 0$. Putting $x = -1$ in the BARW gives $y = -\rho$, defining a dual process with $b' = 1 + \rho$, $c' = 1$, $d' = \rho$. These rates are a combination of those of an annihilating branching process (ABP, $b = c = 1$) (see Sudbury 1990, Bramson *et al* 1991) and a voter model (VM) rate ρ ($b = d = \rho$), so we shall designate it by ABP/VM. $x = -1$ corresponds to an annihilating duality which could be derived by graphical means.

Sudbury (1997b), theorem 4, shows that if the probability an IPS survives from a finite initial set is positive, then the probability of survival will be positive for any dual. Further, it is shown in theorem 1 that any IPS with $b > 0$ is self-dual with parameter $y = 0$ or

$x_{\text{self}} = (d - a - c)/b$. Thus, the BARW is self-dual with parameter $-(1 + 2\rho)$ and the ABP/VM has self-duality parameter $(\rho - 1)/(1 + \rho)$. It follows indirectly from Sudbury and Lloyd (1997), theorem 11 and directly from Sudbury (1997b), theorem 3, that the BARW is a $1/(1 + \rho)$-thinning of the ABP/VM in the sense that if the initial configuration of a BARW is a $1/(1 + \rho)$-thinning of the initial configuration of the ABP/VM, this relationship holds for all subsequent times. Since the chief inaccuracy in the method outlined for the contact process was in the bound put on the number of spaces by which the process could contract when the end 1 died, it is conjectured that the supermartingale method will be more accurate if the IPS with a greater density of particles is used. We illustrate this by comparing the values of ρ for which the ABP/VM dies out to those of the BARW.

There is an immediate pay-off in one dimension when we consider the case $m = 1$. Suppose the left-hand end of the ABP/VM is 11. Then the left-hand 1 branches to the left at rate $1 + \rho$, but the left-hand 1 dies at rate ρ and coalesces at rate 1, so in this situation the rate of change of the expected position of the left-hand 1 is 0.

If the left-hand end is of the form 10 then, as before, the 1 branches to the left at rate $1 + \rho$, but the 1 dies at rate 2ρ and moves at least two spaces to the right. Thus, the rate of change of the expected position is $\leqslant 1 - 3\rho$. Clearly, if $\rho > 1/3$ it is possible to create a supermartingale for the ABP/VM. We therefore have the following lemma.

Lemma 2. When $\rho > 1/3$ in one dimension, the BARW and the ABP/VM have extinction probability 1 when the initial configuration is finite.

The argument when applied to the BARW is more complicated. Assuming a score of 0 when the left-hand end is in state $\ldots 10 \ldots$ and $-s$ when in the state $\ldots 11 \ldots$, the rates of change of the expected changes in score are as follows: first assume the left-hand end is $0100 \ldots$ then the rate of change is $1 - 2s + (\rho - \rho)$. Then assume the left-hand end is $\ldots 111 \ldots$. In this case the rate of change is $2\rho(-2 + s + s) + \rho(1 + s) + 1 + 1(-1 + 2s)$. It is simple to check that for both expressions to be $\leqslant 0$, it is necessary that $s = 1/2$, $\rho \geqslant 2$, confirming in this instance the conjecture that the ABP/VM is more effective to work with.

Because the model is non-attractive there is no obvious candidate for the values to the right of the m-configuration that will be most advantageous. It is clearly impossible to look at all possibilities since they exceed $2^{2^{m-1}}$, but fortunately a straightforward search procedure locates the most advantageous set of configurations relatively rapidly. We consider the BARW.

First, a random set of right configurations is generated. The Q-matrix and the values of $\underline{a}$ corresponding to this set are calculated by the computer program. Put $\underline{S} = -(Q^*)^{-1}\underline{a}$. Then, the special case $i = 2^{m-1}$ is considered as this corresponds to $\ldots 0110000 \ldots$. It is assumed that at rate 2ρ the leftmost pair of 1's annihilate each other and the leftmost 1 moves $m+1$ places to the right. There are 2^m possible right configurations, each defining the m-configuration for the state 2^{m-1} to jump to. The Q-matrix for each of these configurations is calculated. It is only necessary to do this for the q_{ij}, $i = 2^{m-1}$, as this is the only part of the matrix that is being changed. For each of the 2^m possibilities, $\sum q_{ij} S_j + a_i$ is calculated. The right configuration giving the largest value is chosen and a new Q-matrix calculated using that right configuration.

Keeping the same value of $\underline{S}$, the state $i = 0$ is considered. There are only two possibilities here, $x_1 = 0, 1$. The same procedure is carried out. For each of these possibilities a Q-matrix is determined and the corresponding values of $\sum q_{ij} S_j + a_i$ for $i = 0$. Whichever of $x_1 = 0, 1$ performs best is then chosen for the new Q-matrix (which, of course, may be the same as at the end of the last round).

We now go to the state $i = 1$ and repeat the process, and then similarly through all the other states, returning to the beginning, when the cycle starts again with a calculation of $\underline{S} = -(Q^*)^{-1}\underline{a}$ with the new Q. When a complete cycle of $i = 2^{m-1}$ and then $i = 0, \ldots, 2^m - 1$ is performed without the Q-matrix being modified, the procedure is ended. If the final value of $\sum q_{0j}S_j + a_0$ is negative then a supermartingale for the process has been discovered, as lemma 3 will show.

Perhaps unexpectedly, in all the examples tried, the above procedure did terminate, although it has not been proved that it must. Furthermore, in every case the terminal value of $\sum q_{0j}S_j + a_0$ was the same, whatever initial Q-matrix had been randomly chosen.

In what follows it is convenient to describe the state 2^{m-1} as -1 when we are considering the annihilation of the leftmost pair of 1's, and as 2^{m-1} when we are considering the effect of x_1.

Lemma 3. Suppose that there exists a Q-matrix for the process with $\sum q_{ij}S_j + a_i \leqslant 0$ for $i = 0, \ldots, 2^m - 1$. For each state i (including -1), the Q-matrix can be changed by a different choice of right configuration. Suppose there are n_i such choices for i, and call the changed Q-matrices Q^{ik} with corresponding $\underline{a}^{ik}$, $k = 1, \ldots, n_i$. (Note that for one of the values of k, $Q^{ik} = Q$, $\underline{a}^{ik} = \underline{a}$.) If (putting $a_{-1} = a_0$)

$$\sum_j q_{ij}^{ik}S_j + a_i^{ik} \leqslant \sum_j q_{ij}S_j + a_i \tag{2}$$

for every $i = -1, 0, \ldots, 2^m - 1$, $k = 1, \ldots, n_i$ then

$$\sum q_{ij}S_j + a_i \leqslant 0 \Rightarrow \sum q'_{ij}S_j + a_i \leqslant 0$$

for any Q-matrix Q' of the process.

Proof. Once the $\{S_j\}$ are fixed, each inequality for i operates independently of the others. □

Using the procedure outlined above, changepoint values for the BARW and the ABP/VM were calculated for $m = 2, 3, 4, 5, 6, 7, 8$. At $m = 8$ the Vax computer being used was taking around 15 min to find the most advantageous right configurations for each value of b. It would have taken some hours for $m = 9$ and days for $m = 10$, so it was decided to stop at $m = 8$. The results confirm the conjectured better performance for the ABP/VM for lower values of m. The equivalence of the values of ρ is not strictly reached until the case $m = \infty$.

m	ρ_m (ABP/VM)	ρ_m (BARW)
1	0.33	2.0
2	0.285	0.368
3	0.246	0.254
4	0.222	0.225
5	0.205	0.208
6	0.193	0.195
7	0.184	0.185
8	0.176	0.177

It still has not been proved that these values of ρ are bounds on the critical value of the process, since supermartingales have only been found for specific values of ρ. It is,

however, true that in every case tried the final value of $\sum q_{0j} S_j + a_0$ did increase with ρ. This same problem was faced when finding critical values for the BABP (Sudbury 1997a), but this time matters are simpler as it turns out that the supermartingale $\{S_j\}$ found for the ABP/VM with $\rho = 0.176$ is also a supermartingale for $\rho = 0.34$. This was checked by starting with the optimal set of right configurations found for $\rho = 0.176$. These were then used along with $\rho = 0.34$ to create a Q-matrix. Then for each $i = -1, \ldots, 2^{m-1}$, the set of possible Q-matrices Q^{ik} were created and the expression $\sum q_{ij}^{ik} S_j + a_i^{ik}$ calculated. In every case this expression was found to be negative, demonstrating that the $\{S_j\}$ also defined a supermartingale for $\rho = 0.34$. Since each Q-matrix and each $\underline{a}$ is a linear function of ρ, the Q-matrix and $\underline{a}$ for values of ρ between 0.176 and 0.34 are linear combinations (with positive coefficients) of the Q-matrices and $\underline{a}$'s at 0.176 and 0.34. Thus, $\sum q_{ij}^{ik} S_j + a_i^{ik} \leqslant 0$ for every possible i, k, ρ with $0.176 \leqslant \rho \leqslant 0.34$. Combining this result with lemma 2 we obtain the following.

Theorem. In one dimension the BARW dies out when $\rho \geqslant 0.176$.

4. The annihilating random walk with branching $a = 2\rho$, $b = 1$, $e = \rho$

This model is the BARW not allowing coalescence. Using the procedure outlined for the BARW, changepoint values for the ARW with branching were calculated for $m = 3, 4, 5, 6, 7$.

m	ρ_m
3	0.39
4	0.35
5	0.33
6	0.31
7	0.30

It should be noted that, although in every case tried the final value of $\sum q_{0j} S_j + a_0$ did decrease with ρ, it has not been proved that this is the case. ρ_m above is a value of ρ at which the final value was positive, whereas it was negative for $\rho_m + 0.01$. Since coalescence is not allowed in this model, it is to be expected that the 'critical' value of ρ should be larger than for the BARW.

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