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The histogram characteristics of perimeter polynomials for directed percolation

J. A. M. S. Duarte (*)
Solid State Physics, Imperial College, London SW7 2AZ, U.K.

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Abstract. — New perimeter polynomials (in dimensions \( d = 2 \) to 4) are analysed for directed site percolation. A study of these data shows that i) above \( p_c \) the average perimeter-to-size ratio varies as \( a = (1 - p)/p + B_s^{-1/d} \); ii) at \( p_c \) its leading correction term estimates supports the prediction (from scaling) of an exponent equal to \( 1/\theta \) (with \( \theta \) the gap exponent for directed percolation); iii) at \( p = 0 \) the limiting ratio is estimated on various lattices. Fairly definitive evidence is obtained in favour of \( a(p = 0) = 3/4 \) for the square site animals and this result is used to study the second correction term which is estimated to be analytic \( (\sim s^{-2}) \) as the first correction term (Bethe-like and \( \sim s^{-1} \), without any obvious dimensional dependence).

Introduction.

The study of directed systems has been a comparatively late development in the evolution of the percolation and animal problems, although a significant body of knowledge has been accumulating steadily on critical exponents and thresholds for percolation [1, 2], as well as on the growth constants for the total number of directed lattice animals [3].

In analogy with the treatment of the undirected percolation problem the probability of occupying the origin or source site in directed (site) percolation can be partitioned into its possibilities of belonging to a finite connected cluster of \( s \) sites, bounded by a number \( t \) of unoccupied sites, so that if \( g_{st} \) gives the number of configurations rooted at the origin and with a given pair \( s, t \) they will obey the sum rule [4]

\[
p = \sum_{s,t} g_{st} p'(1 - p)^t \quad p < p_c.
\]

It is the structure and asymptotic limiting form of the histograms \( g_{st} \) (as fixed \( s \)) that will be investigated in this paper. Extensive listings can be found in [4] where a detailed description of the procedure adopted in their derivation can be found. The technique is based in the combination of straightforward cluster enumeration and recurrence relations between the \( g_{st} \) at various \( s \) adjacent values.

We have now substantially extended results (1)

(*) On sabbatical leave from : Laboratório de Física, Faculdade de Ciências, Universidade do Porto, 4000 Porto, Portugal.

(1) Available from the author on request.
expanding the current availability of perimeter histograms on most usual lattices in 2 to 4 dimensions: on the square (nearest-neighbour) site problem to $s = 24$ ($s = 17$ in [4]), on the triangular site problem to $s = 17$ ($s = 14$ in [4]), on the simple cubic site problem to $s = 15$ ($s = 12$ in [4]), on the 4-d hyper-cubic site problem to $s = 12$ ($s = 10$ in [4]) and added the body centred cubic and square next-nearest-neighbour site histograms (both to $s = 10$): this is a sufficiently large body of information on which to undertake a comprehensive survey of the histograms $g_s$ across the percolation range and from 2 to 4 dimensions. Section 2 of this paper details the results of a numerical analysis above, at, and below $p_c$. The perimeter polynomials have already been the object of a study at $p = 0$, the so-called animal limit, in reference [5]. These are completed and extended to other lattices and dimensions here and we add results for negative $p (q = 1 - p > 1)$.

2. Numerical analyses.

2.1 Above $p_c$ ($1 > p > p_c$). — This is the region where an infinite cluster always spans from the origin, and gradually occupies the whole lattice as $p \to 1$. In a study of cluster numbers [6] we found that these quantities defined by

$$n_s(p) = p^s \sum g_s(1 - p)^t$$

showed evidence in favour of an essential singularity, characterized by an asymptotic decay with a dimensionally dependent exponent:

$$n_s(p) \sim s^{-\beta} \exp\left(-E_s^{(d-1)/d}\right)$$

this is a result which agrees with the Kunz and Souillard theorem established for undirected percolation [7]. Associated with the asymptotic form (3) for the cluster numbers Kunz and Souillard proved the corollary that the average percolation perimeter defined as

$$\langle t \rangle = \sum_t g_s(1 - p)^t \sum_t g_s(1 - p)^t$$

varied like

$$\langle t \rangle = \frac{1 - p}{p} s + B \ s^{1-1/d} \quad \text{for large } s$$

their argument was crucially based on a set of compact configurations with a vanishing perimeter/size ratio, the squares, which are also present in the fully directed problem (see Fig. 1a): notice however that there is no correspondence between the $g_s$ in both percolation problems — in fact, the directed configurations are a more restricted set, and a graph like figure 1b does not exist in square site directed percolation, although it is present in undirected percolation.

![Fig. 1. — Graphs on the square lattice: a) represents an embedding on the fully directed acyclic square lattice of a compact square: $s = 9$, $t = 6$; b) is an example of a graph which can be embedded in the undirected lattice.](image)

We have analysed the sequences for $\langle t \rangle$ from weighted histograms (Eq. (4)) using the ratio method to estimate the correction to the leading dependence in equation (5) (for a full description see [8] sections 2 and 5, respectively) as well as a fitting formula with 3 parameters $\alpha$, $\beta$, $\xi$

$$\langle t \rangle = \alpha s + \beta s^{1-\xi} + \cdots$$

typical results on 2 and 3 dimensional lattices are shown graphically in figure 2. Good evidence on the triangular lattice in favour of a limiting $\xi = 1/d = 1/2$, was also obtained. The 3 dimensional results suffer from great irregularities for $p > 0.85$ although an improved pattern consistent with $\xi = 1/3$ can be found in the region $0.6-0.45$ for both the simple cubic and the body-centred cubic polynomials. Fitting a formula like (6) improves the sequences for $\alpha$ and brings them

![Fig. 2. — Estimates for the first order correction to the average perimeter-to-size ratio: A) averages of successive ratio method estimates on the s. cubic at $p = 0.80$; A') successive ratio estimates for the same lattice at $p = 0.55$; (common limit 1/3 marked with an arrow on the vertical axis); B) corresponding sequence for the square case at $p = 0.55$, tending to 1/2 (also marked on the vertical axis); C) ratio estimates at $p_c = 0.7055$ [1] for $1 - \sigma = \text{the interval prediction indicated on the vertical axis} 1 - \sigma = 0.61 \pm 0.01.$](image)
closer to \((1-p)/p\), but the evolution of \(\zeta\) is less smooth than the estimates from the ratio method (where \(\alpha = (1-p)/p\) is assumed from the start). Ratio sequences point slightly under \(1/d\) (in all dimensions) while fittings are more irregularly scattered.

We consider there is a good measure of support — particularly convincing for the two-dimensional very long polynomials, in favour of the extension to directed percolation of the asymptotic limiting formula (5).

These conclusions are equivalent to the assumption that in the limit, the \(g_s\) behave like \(\left(\frac{s + t}{t}\right)\) as far as their leading behaviour is concerned. Consider the smoothing out of the \(g_s\) obtained by adopting a variable \(a = t/s\), the perimeter-to-size ratio. Then, \(g_s \to g_s(a)\) and the partial summation in \(t\) goes into an integral in \(a\):

\[
\sum_t g_s p(1-p)^t \to \int g_s(a) p(1-p)^a da. \tag{7}
\]

Keeping in mind that the \(\sum g_s\) are supermultiplicative [3], \(g_s(a) \sim \exp(sA(a))\) and clearly the leading contribution for the integral in equation (7) comes from the point where \(\exp[sA(a) + a \log(1-p)]\) is a maximum. This occurs at \(a = (1-p)/p\) and \(sA(a)\) must be of the form

\[
sA(a) = [(a + 1) \log(a + 1) - a \log a] s \tag{8}
\]

which is the leading term in the logarithm of \(\left(\frac{s + t}{t}\right)\), after using Stirling’s approximation for the factorials. Of course, inside this region \((p > p_c\) equivalent to \(a < a_c\)) equation (1) is not applicable, because the infinite cluster is always present. Below \(p_c\), the double summation in \(s\) and \(t\) of the \(g_s\) verifies equation (1) : this is already some indication that \(A(a)\) for \(a > a_c\) (sometimes called the log multiplicity [8]) must be smaller than equation (8), and correction terms (linear in \(s\)) must be present.

2.2 At the percolation threshold. — At \(p_c\) the low-density sum rule (Eq. (1)) breaks down and

\[
\left| g_s(a) (1-p)^t \right|^{1/s} = 1 \quad (s \gg t \text{ and } s \to \infty) \tag{9}
\]

using the log multiplicity from (8)

\[
a_c = (1-p_c)/p_c
\]

and in the limit \(s \to \infty\)

\[
g_s(a_c) \sim \left[ (a_{c+1})^{a_{c+1}}/a_{c}^{a_{c}} \right] s \tag{10}
\]

these conclusions are once again in line with those found for undirected percolation. From our above mentioned study of cluster numbers [6] we expect to find a correction term that shows explicitly a first order correction of the type (see [9] section 4.1 for what remains the most clear exposition on the cluster perimeter at the percolation threshold : the argument applies, mutatis mutandis, to the present case of directed percolation)

\[
\langle t/s \rangle = \langle a \rangle = (1 - p_c)/p_c + D s^{-1} + \cdots \tag{11}
\]

with the inverse gap exponent, \(\sigma = 1/\Delta, \Delta = \beta + \gamma\).

When \(p_c\) is known exactly \(\sigma\) can be found by simple ratio methods from (11) (see, for example Ref. [8]). For directed percolation, however \(p_c\) is not known exactly and fitting a 3-point formula like (11) or scanning the existing estimate ranges for \(p_c\) while estimating \(\sigma\) is the only alternative. Assuming \(p_c = 0.7055\) as a central value for the square site problem, the ratio estimates for \(\sigma - 1\) are plotted against \(1/s\) in figure 2. The range for \(\sigma - 1\) taking into account the uncertainty in \(p_c\) is indicated on the axis by a *. \(\sigma - 1 = -0.61 \pm 0.01\), in good agreement with the result from a combination of the \(\gamma\) and \(\beta\) values in two dimensions [1], of \(\sigma - 1\) between \(-0.612 - 0.603\). For the simple cubic problem in three-dimensions we have scanned an interval for \(p_c\) rather more reduced than the published estimate [2]. With \(p_c = 0.435 \pm 0.003\) our value of \(\sigma - 1\) is \(-0.54 \pm 0.025\), against an indirect prediction through scaling from \(\gamma\) and \(\beta\) values [2] of between \(-0.550\) and \(-0.524\).

Both the two and three dimensional results are sufficient to show the significant change from a dimensionally dependent correction above \(p_c\) to this scaling related exponent (in undirected percolation studies the corresponding term was sometimes referred to as the « excess perimeter » at \(p_c\) [9]).

2.3 Below \(p_c (p < p_c)\). — Near \(p_c\) a gradual change occurs to the animal limit, with the scaling effects manifest in the \(s^{-1}\) correction in equation (11), disappearing in a 0.10-0.15 range below the critical threshold for all lattices. In a previous pilot study on directed animals \((p = 0\) in Eq. (4))[5], we have reported on Bethe-like limiting behaviour for two-dimensional lattices and the numerical analyses on the present much expanded evidence are shown in table I(2) where a fitting formula of the type

\[
\langle t/s \rangle_{p=0} = a_0 + B s^{-1} \tag{12}
\]

was assumed. The results show a clear uniformity of evolution compatible with a Bethe-like limit \((\sigma^* = 0\) in all cases. The final section of the analyses for the square site problem is given in table II. If \(\sigma^* = 0\), then

\footnote{Footnote : The additional term in some sequences on table I is obtained by a combination of the sum rule (1) with the existing knowledge of \(\sum g_s\) for \(s + 2\). By expanding the \(g_s\) though order \(s + 2\) (following (1)) the coefficient of the \(s + 2\) — term is given by \(- \sum g_{s+2} + \sum g_{s+1} g_{s+1}\). This last value can be added to the histogram averages.}
the first correction to the perimeter-to-size-ratio is analytic and Neville extrapolants are a good, reliable tool. This is brought out by the analyses in table II, where the estimates for \( a_0 \) from a fitting formula like equation (12) are also given. The regularity of even the cubic extrapolants is quite remarkable and as good as good an indication of a limiting \( a_0 = 3/4 \) exactly as could be desired. Our estimates for \( a_0 \) in the various lattices are given in table III.

We have returned to the square site directed animals and used the data to estimate the second correction term under the assumption that

\[
\langle t/s \rangle = 3/4 + Bs^{-1}(C + Cs^{-\varphi} + \cdots) \quad (13)
\]

\( p = 0 \)

The results of such a study are given in table IV and they show clearly that the \( \varphi \) sequences are compatible with a \( \varphi = + 1 \) limit, so that the correction term might
be analytic. Our estimate for $B$ is

$$B = 1.8437 \pm 0.0015. \quad (15)$$

When the first studies on the average perimeter-to-size ratio were discussed [9, 8] the behaviour in the non-critical region was explained by suitable corrections to the log multiplicity, valid only for $a > a_c$.

$$A(a) = (a + 1) \log(a + 1) - a \log a - f(a) \quad (15)$$

so that when inserted into equations (4) and (7), $A(a)$ would lead to a slower evolution of the average $a$, peaking at $a = a_0$ for $p = 0$ where

$$\log \frac{a_0 + 1}{a_0} = f'(a_0) \quad (16)$$

according to the steepest descents method. According to the workers in the field (see, for a detailed review, [9] chap. 5), $f(a)$ should be taken as a power law in the distance to the critical ratio

$$f(a) = c(a - a_0)^\gamma \quad (17)$$

but even as a mimic for those lattices where $a_c$ and $a_0$ are very close this assumption fails in the one very important respect that it cannot accommodate the infinite derivative of the log multiplicity near the maximum value of $a$ (in the present problems this $a_{\text{max}} = d - 1$ for the simple $d$-hypercubic site cases, $a_{\text{max}} = 2$ for the triangular, and 3 for the square n.n.n. and b.c.c. site animals). For square site animals, with the suggestions made earlier, $f'(a)$ must be such that:

$$f(a_0) = 0 \quad (18a)$$

At $a_0 = 3/4$ the log multiplicity is given by $\log \lambda$, with $\lambda = 3$ (Ref. [3])

$$A(3/4) = \log 3 \quad (18b)$$

Equation (16) becomes

$$\log(7/3) - f'(3/4) = 0 \quad (18c)$$

and with $a_{\text{max}} = 1$, the maximum perimeter configurations are self-avoiding walks whose number is $2^z$, so that

$$A(1) = \log 2 \quad (18d)$$

while the log derivative near this maximum implies, as mentioned above

$$A'(1) = -\infty. \quad (18e)$$

A simple power law is clearly inadequate. Rather than trying several alternatives in agreement with equations (18) we have used the perimeter polynomials to study the histogram evolution beyond $a_0$ — i.e. beyond $1 - p = 1$. The results are sufficiently well behaved for meaningful extrapolation to a limiting perimeter-to-size ratio and we have tabulated the asymptotic approach to $a_{\text{max}}$ in table V. The varying estimate ranges reflect the fluctuating range of exponents of the first order correction which get very close to 1 (until around $1 - p = 8$) and then return to non-monotonic sequences below the animal ($p = 0$) sequences of table I.

Table V. — Estimates of the perimeter-to-size ratio for $1 - p$ values beyond the animal limit.

<table>
<thead>
<tr>
<th>$1 - p$</th>
<th>Limiting $a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3/4</td>
</tr>
<tr>
<td>1.2</td>
<td>0.777 ± 0.001</td>
</tr>
<tr>
<td>1.3</td>
<td>0.7885 ± 0.0015</td>
</tr>
<tr>
<td>1.4</td>
<td>0.798 ± 0.001</td>
</tr>
<tr>
<td>1.7</td>
<td>0.821 ± 0.001</td>
</tr>
<tr>
<td>2.0</td>
<td>0.838 ± 0.0015</td>
</tr>
<tr>
<td>3.0</td>
<td>0.8725 ± 0.0015</td>
</tr>
<tr>
<td>4.0</td>
<td>0.8925 ± 0.001</td>
</tr>
<tr>
<td>5.0</td>
<td>0.9058 ± 0.001</td>
</tr>
<tr>
<td>8.0</td>
<td>0.928 ± 0.002</td>
</tr>
<tr>
<td>10.0</td>
<td>0.936 ± 0.003</td>
</tr>
<tr>
<td>12.0</td>
<td>0.943 ± 0.003</td>
</tr>
<tr>
<td>15.0</td>
<td>0.949 ± 0.003</td>
</tr>
<tr>
<td>20.0</td>
<td>0.958 ± 0.004</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$\infty$</td>
<td>1</td>
</tr>
</tbody>
</table>


The histograms of directed site percolation polynomials reveal a limiting structure associated with the occurrence of an essential singularity above $p_c$, with an average perimeter-to-size ratio given by $a = (1 - p)/p$ in the limit and a dimensionally dependent first correction (Eq. (6)). At the percolation threshold the first correction has been estimated in two and three dimensions and shown to be in agreement with scaling, leading to an exponent $\sigma - 1$ where $\sigma = 1/J (A$, the gap exponent). Inside the non-critical zone each lattice was analysed for the most important characteristics of the perimeter histograms, leading to the estimation of their perimeter-to-size ratio for $p = 0$ (animal limit). On the square lattice the quality and extension of the data was used to study the correction terms of second order, with the conclusion that the first two corrections are likely to be analytic.

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References