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Numerical calculations of critical densities for lines and planes

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Abstract. Critical percolation densities have been calculated numerically for large systems of lines in two dimensions and planes in three dimensions. Results for lines of varying length have been successfully predicted from the constant length case. In special cases very large systems of up to $\frac{1}{4}$ million lines have been studied. By calculating critical densities for a range of system sizes and using a finite-size scaling argument, a prediction of the infinite critical density is made. For the two-dimensional system with fixed length orthogonal lines this corresponds to 3.11 intersections per line. For the three-dimensional system of fixed size orthogonal planes, the prediction is 2.00 intersections per plane.

1. Introduction

The critical density for percolation in some systems of line segments in two dimensions was calculated numerically and reported by the author (Robinson 1983). We shall subsequently refer to this as paper I. Some results have also been obtained by Balberg and Binenbaum (1983). Both studies used small systems of around 1000 lines. The computer program used in I has now been improved and implemented on the CRAY-1S computer. This has enabled much larger systems to be used. Three-dimensional systems of square planes have also been looked at. For special cases we have been able to use systems with over 250 000 lines or 200 000 planes. By looking at the way the calculated critical density varies with increasing system size and using a finite-size scaling argument we can predict the infinite results with some confidence.

2. Numerical calculation

For numerical calculation of critical densities in two dimensions we use the following technique. We take a square region and generate lines randomly in and around it. The lines are uniformly distributed in space and have the specified length and orientation distributions. Each new line can

(i) form a new cluster (no intersections)
(ii) extend an existing cluster
(iii) unite two or more existing clusters.

After each line we check modified clusters to see if they satisfy the percolation criterion (generally this requires the cluster to connect all four sides of the region). Once the criterion is satisfied line generation is stopped and the critical density recorded.

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The most time consuming part of the calculation is finding which lines intersect. We have developed an algorithm which does this very quickly and so allows large systems to be used. The basic technique is to cover the region with a square grid, and to maintain a list of lines which pass through each grid block. Only lines which pass through a common grid block can possibly intersect. The block size can be chosen to optimise the algorithm, we have found that having two or three lines per block gives the best results.

In three dimensions this can be extended in the obvious way to deal with planes.

In order to deal with very large systems further improvements in the algorithm were necessary. These were possible in the special case of fixed size orthogonal systems, both in two and three dimensions. In these cases we can make two improvements. The block size can be chosen so that the lines are exactly two blocks long, then the blocks through which a line passes can be found very quickly. Also all intersections involve one line in each direction, so by keeping separate lists for the two directions the number of checks to be made can be halved. With all these improvements the program can find $\frac{2}{3}$ million intersections per second. The restriction on system size is the memory capacity of the computer.

3. Results of large runs for general cases

3.1. Case I

In this case the lines are all of fixed length two units, with orientations distributed uniformly in the interval $(-\alpha, \alpha)$, for various α. In each case 50 realisations were used. The region used was 80 units square so there were over 9000 lines in each realisation. Table 1 gives the results, the final column being from the theoretical relationship derived in I.

Table 1. Results for case I, uniform distribution of orientations.

α	Density ρ Average	Density ρ Std dev.	Intersections I Average	Intersections I Std dev.	$\frac{\langle I\rangle}{\langle\rho\rangle}$	$\frac{2}{\alpha^2}(2\alpha-\sin 2\alpha)$
90°	1.434	0.0624	3.650	0.1568	2.545	2.546
80°	1.452	0.0509	3.650	0.1331	2.514	2.514
70°	1.498	0.0410	3.615	0.1091	2.413	2.413
60°	1.612	0.0618	3.606	0.1433	2.237	2.240
50°	1.795	0.0767	3.582	0.1559	1.996	1.997
40°	2.126	0.0835	3.590	0.1481	1.689	1.688
30°	2.728	0.1301	3.607	0.1700	1.322	1.322
20°	4.002	0.1495	3.639	0.1417	0.909	0.908

It can be seen that the average density and average number of intersections are related as predicted and that the average number of intersections at percolation is decreasing slightly as α decreases. It should be remembered that more lines are present in the fixed size region for smaller α and so the finite-size effects account for some of this decrease. For the smallest α values the number of intersections increases again. We will see in the next example that this occurs even when we know that it must be constant. It must therefore be due to the finite size region, and in particular the aspect ratio of this region as compared to the spread of angles. The region is effectively much wider at small α and so the calculated percolation density is increased.

3.2. Case II

The second example was for the case with a fixed length of 2 units and orientations at $\pm\alpha$ from the horizontal. As Balberg and Binenbaum (1983) have pointed out in this case the number of intersections is independent of α. The results presented in table 2 are for 50 realisations with over 10 000 lines in each case. The final column is the theoretical relationship derived in I.

Table 2. Results for case II, bimodal distribution of orientations.

	Density ρ		Intersections I		$\frac{\langle I\rangle}{\langle\rho\rangle}$	
α	Average	Std dev.	Average	Std dev.		$2\sin 2\alpha$
45°	1.587	0.0565	3.171	0.1131	1.998	2.000
40°	1.616	0.0605	3.175	0.1149	1.965	1.970
35°	1.685	0.0569	3.161	0.1052	1.876	1.879
30°	1.835	0.0685	3.178	0.1160	1.732	1.732
20°	2.526	0.0867	3.248	0.1134	1.286	1.286

Again the relationship between the average number of intersections and the density is as predicted. I_c is constant, as predicted, except for the smallest angle. This is the same as for the previous example, presumably being due to the effective width increase for small α.

3.3. Case III

In this case we look at the way variability in line lengths affects the critical density. The lines are oriented in uniformly random directions and their lengths are uniformly distributed in the interval $(2(1-\theta), 2(1+\theta))$ for a range of θ between 0 and 1. The predicted behaviour derived in I was that density would be proportional to $(1+\frac{1}{3}\theta^2)^{-1}$. The ratio between intersections and density is predicted to be a constant with value $8/\pi = 2.546$.

The average number of intersections over the density is consistently close to the theoretical value. The predicted change in critical density is close to the calculated

Table 3. Results for case III, uniform distribution of line lengths.

	Density ρ		Intersections I		$\frac{\langle I\rangle}{\langle\rho\rangle}$	
θ	Average	Std dev.	Average	Std dev.		$\rho(1+\frac{1}{3}\theta^2)$
0.0	1.434	0.0624	3.650	0.1568	2.545	1.434
0.2	1.428	0.0532	3.640	0.1325	2.549	1.447
0.4	1.370	0.0614	3.493	0.1568	2.550	1.443
0.6	1.301	0.0469	3.320	0.1143	2.552	1.457
0.8	1.207	0.0523	3.077	0.1318	2.549	1.464
1.0	1.095	0.0304	2.788	0.0952	2.546	1.460

value, giving an error of around 2%. For the large values of θ there are less lines generated so the finite size-effects will push up the calculated density and explain some of the discrepancy.

3.4. Case IV

In this case we take a different line length variation. This time the lines have lengths 2 or $2l$ with equal probability. l is taken between 0 and 1.2. In each case 50 realisations were done. The results are presented in table 4. The theoretical prediction is that $\rho(1+l^2)/2$ is constant, and that the ratio between intersections and density is $(2/\pi)(1+l)^2$. These values are given in the table.

Table 4. Results for case IV, bimodal distribution of line lengths.

l	Density ρ Average	Std dev.	Intersections I Average	Std dev.	$\frac{\langle I\rangle}{\langle\rho\rangle}$	$\rho\frac{(1+l^2)}{2}$	$\frac{2}{\pi}(1+l)^2$
0.0	2.868	0.1248	1.825	0.0748	0.636	1.434	0.637
0.2	2.810	0.0945	2.577	0.0958	0.917	1.461	0.917
0.4	2.529	0.0879	3.158	0.1102	1.248	1.467	1.248
0.6	2.128	0.0885	3.470	0.1488	1.630	1.447	1.630
0.8	1.748	0.0675	3.604	0.1397	2.063	1.433	2.063
1.0	1.434	0.0624	3.650	0.1568	2.546	1.434	2.546
1.2	1.178	0.0463	3.633	0.1438	3.081	1.437	3.081

The $l=0$ result here was not actually calculated separately but was deduced from the $l=1$ case. The theoretical result again seems to work well in these cases. The least good results are for $l=0.2$ and $l=0.4$ although even these are only 2% in error.

3.5. Case V

This is a three-dimensional case. We took unit squares with uniformly distributed orientations in a region 20 by 20 by 20, so that there were around 10 000 squares for each realisation. The average over 50 realisations gave an average critical density of 1.231 planes per unit volume with an average of 2.461 intersections per plane. A ratio of 2.0 between these figures is predicted from geometrical considerations.

3.6. Summary of results

These results have shown that the relationship between intersection number and density is exactly as predicted, confirming that the program is finding all the intersections. For cases with varying line length the average intersections per line is not constant. If a weighted average is taken with the weight being the line length this is almost constant and so the critical density can be predicted.

4. Region size effects

4.1. Finite-size scaling

In numerical calculations only finite systems can be considered. If we wish to find the critical density for infinite systems we must extrapolate from the finite-size results.

In this section we deduce the form of the critical density against region size curve from finite-size scaling arguments (Fisher 1971).

Let R be the region size, C be the correlation length (which diverges at the transition) and ρ be the density which has critical value ρ_c in the infinite case. Then C is a function of ρ and R. For ρ near ρ_c and infinite R the correlation length has the form

$$C(\rho, \infty) \propto (\rho - \rho_c)^{-\nu}$$

where ν is the correlation length exponent. This is known to be $\frac{4}{3}$ for two-dimensional lattices (Essam 1980). In a finite system criticality is reached when $R/C(\rho, \infty)$ is some constant, i.e. when $R(\rho - \rho_c)^{\nu}$ is constant. So

$$(\rho - \rho_c) \propto R^{-1/\nu}.$$

This gives a relationship

$$\rho_c(R) = \rho_c(\infty) + aR^{-3/4}$$

if the lattice value for ν is assumed. In three dimensions the argument is the same but $\nu = \frac{4}{5}$.

4.2. *Results for the two-dimensional case*

The case considered was for two orthogonal line sets oriented parallel to the sides of the region. In all cases the lines were of length 2 units, the region size ranged from 10 units to 400 units. For each region size at least 100 realisations were done, the actual number done in each case is given in table 5. The number of lines in the table refers to the number generated in an extended area around the region, 1 unit larger

Table 5. Results of region size variation runs in two dimensions.

Box size	Number of runs	Number of lines Average	Number of lines Std dev.	Density Average	Density Std dev.	Time per run (s)	Time per run per line (μs)
10	400	233	33.9	1.616	0.2355	0.0053	22.77
20	400	775	69.5	1.600	0.1436	0.0176	22.71
30	400	1640	119.9	1.602	0.1171	0.0381	23.23
40	400	2799	168.9	1.587	0.0958	0.0658	23.51
50	500	4285	208.3	1.585	0.0770	0.101	23.57
60	100	6102	284.1	1.587	0.0739	0.144	23.60
70	100	8179	326.5	1.578	0.0630	0.194	23.72
80	100	10 627	418.0	1.580	0.0622	0.254	23.90
90	100	13 422	346.7	1.588	0.0410	0.319	23.77
100	200	16 369	467.8	1.573	0.0450	0.391	23.87
110	100	19 807	609.6	1.579	0.0486	0.477	24.08
120	100	23 456	548.5	1.576	0.0369	0.563	24.00
130	100	27 326	668.7	1.568	0.0384	0.654	23.93
140	100	31 544	751.2	1.564	0.0373	0.754	23.90
150	100	36 216	834.3	1.568	0.0361	0.877	24.17
200	200	63 896	1050.5	1.566	0.0257	1.559	24.37
250	100	99 468	1489.1	1.566	0.0235	2.414	24.27
300	200	142 310	2010.0	1.560	0.0220	4.480	31.42
400	200	252 212	2854.2	1.561	0.0177	7.952	31.51

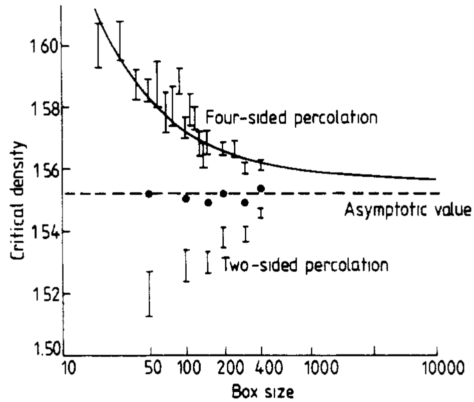

Figure 1. Critical density against box size for orthogonal lines of length 2 units. The full circles show the average of the two criteria and the full curve shows the finite-size scaling fit.

in each direction. This area was used since lines centred within it could enter the percolation region. The time per realisation is given and the time per realisation divided by the average number of lines. This shows that the algorithm used takes a time which increases only linearly with the number of lines. The sudden increase for the largest two region sizes is due to a change in algorithm to reduce the amount of computer space used so that the code would fit into the CRAY-1S at Harwell.

The best least squares fit to the results gives $\rho_c(\infty) = 1.556$ with $a = 0.505$. This is shown on figure 1 with all the results, including some results for runs where the percolation criterion was relaxed to count any cluster connecting two opposite sides as percolating. These runs are summarised in table 6.

It can be seen that the reduction in calculated critical density caused by changing the criterion is approximately equal to the standard deviation of the critical density. It is clear that the average between old and new densities is very nearly constant, suggesting that the two densities are tending towards this value at equal rates. The previous estimate, using the finite-size scaling with $\nu = \frac{4}{3}$ gave $\rho_c = 1.556$ which agrees very closely with this average value of 1.552. It seems plausible that the four-sided criterion overestimates critical densities and the two-sided criterion underestimates them. Taking all the results together there seems little doubt that the true critical density in this case is very close to 1.556, with 3.112 intersections per line.

As the region size increases the standard deviation in the density at percolation goes down, it must be zero for infinite regions. In figure 2 we plot the logarithm of

Table 6. Comparison of original percolation criterion and two-sided criterion.

Box	Four sides density		Two sides density		Change in	Average
size	Average	Std dev.	Average	Std dev.	density	density
50	1.585	0.0770	1.520	0.0707	0.065	1.5525
100	1.573	0.0450	1.529	0.0483	0.044	1.5510
150	1.568	0.0361	1.530	0.0331	0.038	1.5490
200	1.566	0.0257	1.538	0.0306	0.028	1.5520
300	1.560	0.0220	1.539	0.0215	0.021	1.5495
400	1.561	0.0177	1.546	0.0151	0.015	1.5535

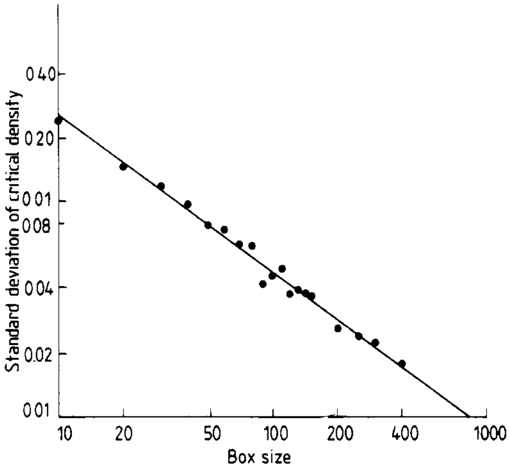

Figure 2. Standard deviation of critical density against box size of orthogonal lines of length 2 units.

the standard deivation against the logarithm of the region size. The best fit line is shown. This gives the relationship $\sigma_c(R) = 1.3R^{-0.722}$ which gives a very good fit. The exponent in this is very close to $-\frac{3}{4}$ suggesting that the variability in the percolation density is proportional to the discrepancy between the finite and infinite critical densities, i.e. $\sigma_c(R) = 2.57(\rho_c(R) - \rho_c(\infty))$.

4.3. *Results in three dimensions*

In this case planes 1 unit by 1 unit were used in regions up to 50 by 50 by 50. The planes all had sides parallel to one of the coordinate axes and were parallel to a coordinate plane. Two percolation criteria were used, the first required a cluster connecting any pair of opposite faces of the cube, while the second required a cluster connecting all six faces. Table 7 presents the results. In each case 100 realisations were done, except for the largest cube for which 50 realisations were done. In all cases the time taken per plane per realisation was just less than 60 μs.

Table 7. Comparison between original percolation criterion and two-faces criterion.

		Six faces		Two faces			
Cube size	No of fractures	Density Average	Density Std dev.	Density Average	Density Std dev.	Difference	Average
10	2197	0.2064	0.0131	0.1842	0.0134	0.0222	0.1953
15	6536	0.1995	0.0087	0.1830	0.0091	0.0165	0.1913
20	14 593	0.1970	0.0057	0.1855	0.0069	0.0115	0.1913
25	27 282	0.1940	0.0054	0.1845	0.0063	0.0095	0.1893
30	45 921	0.1927	0.0039	0.1853	0.0051	0.0074	0.1890
35	71 496	0.1916	0.0034	0.1856	0.0040	0.0060	0.1886
40	105 398	0.1912	0.0030	0.1857	0.0030	0.0055	0.1885
45	148 094	0.1902	0.0024	0.1854	0.0027	0.0048	0.1878
50	201 906	0.1903	0.0022	0.1856	0.0028	0.0047	0.1879

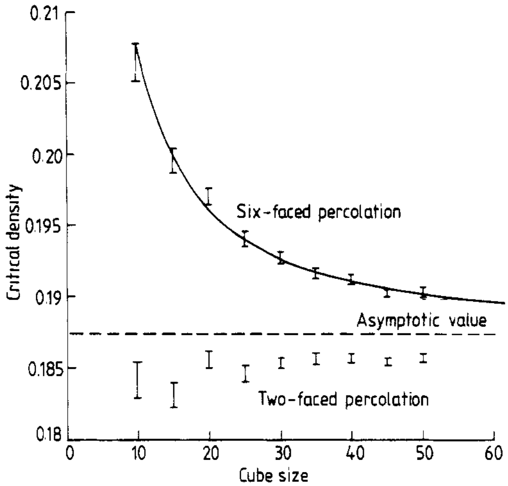

Figure 3. Critical density against box size for orthogonal planes of size 1 unit by 1 unit. The solid line shows the finite-size scaling fit.

The pattern of results is similar to the two-dimensional case, with the two definitions of percolation giving results that get closer as cube size increases. The scaling argument this time predicts a decrease with $C^{-5/4}$, where C is the cube size. A least squares fit to the results gives a limiting value of 0.1874, in good agreement with the trend of the average results. This limit corresponds to an average number of intersections of almost exactly 2.0. Figure 3 shows all these results.

5. Conclusions

The predicted critical densities for lines in two dimensions have been improved. New results are given for planes in three dimensions. The infinite results for two particular systems, the orthogonal cases in two and three dimensions, have been predicted with the help of finite-size scaling arguments and some very large calculations. The two-dimensional case percolates when there are 3.11 intersections per line. In three dimensions 2.00 intersections per plane are required.

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