On the asymptotic number of lattice animals in bond and site percolation

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Abstract. A recently proposed asymptotic form, due to Domb, for the total number of bond and site animals of size n, has been investigated numerically. It is found to fit the available data better than simpler forms previously assumed. The critical parameters entering into the asymptotic form are estimated for a number of two- and three-dimensional lattices, and conclusions are drawn about their lattice and dimensional dependence. In particular, the cluster growth parameter λ is estimated with a higher degree of precision than that previously attained.

1. Introduction

For a wide variety of lattice models, the method of exact series expansions typically provides the first dozen or so coefficients of some generating function of interest. Analysis of these coefficients is then performed in order to determine the asymptotic form either of the coefficients or their generating function. The success of this procedure clearly depends on the available coefficients displaying the appropriate asymptotic behaviour.

The most common asymptotic form assumed is $c_n \sim A\mu^n n^g$, where c_n is the nth coefficient of the generating function $C(x) = \sum_{n \geq 0} c_n x^n$, μ is a lattice and model dependent constant and g is an exponent which characterises the nature of the singularity in the generating function at $1/\mu$.

Recently Sykes and Glen (1976) and Sykes *et al* (1976) analysed the generating function for the total number of clusters, commonly known as the 'animal' generating function, both for the bond and the site problems. Reference should be made to these papers and Essam (1972) for a full description of the problem. The only rigorous result is that due to Klarner (1967) who showed that the animals were multiplicative, and hence that the number of animals of size n is given by $c_n \sim \lambda^n \phi(n)$, where $\lim_{n \to \infty} (\phi(n))^{1/n} = 1$.

The asymptotic form was assumed by Sykes and Glen (1976) and Sykes *et al* (1976) to be $c_n \sim A\lambda^n n^{-\tau}$ as usual, and their results, while not inconsistent with this assumption, did not show the rapid rate of convergence observed for other lattice problems, such as the Ising and self-avoiding random walk models. This is reflected in the comparatively large error bounds cited for the parameters λ and τ. Subsequently, Domb (1976) suggested that the appropriate asymptotic form for the total number of

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animals was more complex than that appropriate to the Ising model, since only ramified clusters made a significant contribution. Domb argued that the appropriate asymptotic form was $c_n \sim A\lambda^n n^{-\tau} \exp(-Fn^{1-\theta})$, and suggested that the presence of the exponential term may explain the slow convergence observed by Sykes and Glen (1976) and Sykes *et al* (1976). The results that follow from this suggested form are determined in the remainder of this paper.

2. Analysis of animal series

We have investigated Domb's proposal by fitting successive quintuples of coefficients, $c_i, c_{i-1}, \ldots c_{i-4}$ to the expression $A\lambda^n n^{-\tau} \exp(-Fn^{1-\theta})$ in order to determine the five unknown parameters A, λ, τ, F and θ, which involves solving a system of non-linear equations. Fortunately however, only θ enters non-linearly, and once this is determined, all the other parameters may be readily obtained by simple algebra. This is repeated for successive quintuples of coefficients, thus providing a sequence of estimates of the unknown parameters. Typical results for site animals per site of a triangular lattice are shown in table 1. The first column, labelled 'N', refers to the last coefficient used in the quintuple. It can be seen that λ has settled down to a very stable value, from which we estimate $\lambda = 5 \cdot 183 \pm 0 \cdot 001$ while the sequence estimating τ is reasonably well converged also, and we estimate $\tau = 1 \cdot 00 \pm 0 \cdot 01$. The other parameters are not as well converged, and we estimate $\theta = 1 \cdot 7 \pm 0 \cdot 2$, $F = 0 \cdot 36 \pm 0 \cdot 03$ and $A = 0 \cdot 28 \pm 0 \cdot 02$. The analysis of Sykes and Glen (1976) gave the estimates τ 'very close to unity' and $\lambda = 5 \cdot 19 \pm 0 \cdot 03$. The results given here are therefore substantially better converged, at least for this lattice. We have repeated this procedure for other lattices in both two and three dimensions. In table 2 we summarise our results for site animals. Before discussing these results further, we will turn our attention to the bond animal generating function, where each coefficient represents the number of bond animals per bond of the lattice. The results of a five parameter fit are shown in table 3 for the same lattices as in the site problem. For both site and bond animals we find that the sequence of estimates of λ is well converged, those for τ reasonably well converged, while sequences for the other parameters are less well converged. In some cases we have not felt confident to extrapolate a sequence, either because the available series is too short or because the sequence of estimates is too erratic to extrapolate confidently. These cases have been indicated by a dash in the table entry.

Table 1. Five parameter fit to triangular lattice site animals assuming $c_n = A\lambda^n n^{-\tau}$ $\times \exp(-Fn^{1-\theta})$.

N	θ	λ	τ	F	A
10	2·095	5·179	0·973	0·292	0·251
11	2·106	5·179	0·972	0·291	0·251
12	1·577	5·185	1·024	0·436	0·307
13	1·852	5·1820	0·991	0·325	0·266
14	1·696	5·1832	1·006	0·363	0·282
15	1·694	5·1832	1·006	0·364	0·283
16	1·694	5·1832	1·006	0·364	0·283
Extrapolated limit	1·7±0·2	5·183±0·001	1·00±0·01	0·36±0·03	0·28±0·02

Table 2. Results of a five parameter fit to two- and three-dimensional site animals/site.

Lattice	τ	λ	θ	F	A
Square	$1 \cdot 0 \pm 0 \cdot 2$	$4 \cdot 065 \pm 0 \cdot 005$	$1 \cdot 4 \pm 0 \cdot 3$	—	—
Triangular	$1 \cdot 00 \pm 0 \cdot 01$	$5 \cdot 183 \pm 0 \cdot 001$	$1 \cdot 7 \pm 0 \cdot 2$	$0 \cdot 36 \pm 0 \cdot 03$	$0 \cdot 28 \pm 0 \cdot 02$
Simple cubic	$1 \cdot 45 \pm 0 \cdot 05$	$8 \cdot 33 \pm 0 \cdot 02$	$< 2 \cdot 8$	$< 1 \cdot 0$	$0 \cdot 17 \pm 0 \cdot 03$
Body-centred cubic	—	$11 \cdot 2 \pm 0 \cdot 2$	—	—	—
Face-centred cubic	$1 \cdot 5 \pm 0 \cdot 1$	$13 \cdot 94 \pm 0 \cdot 05$	$1 \cdot 8 \pm 0 \cdot 3$	$0 \cdot 6 \pm 0 \cdot 2$	$0 \cdot 12 \pm 0 \cdot 03$

Table 3. Results of a five parameter fit to two- and three-dimensional bond animals/bond.

Lattice	τ	λ	θ	F	A
Square	$0.96 \pm 0 \cdot 1$	$5 \cdot 25 \pm 0 \cdot 1$	—	—	$0 \cdot 25 \pm 0 \cdot 03$
Triangular	$1 \cdot 00 \pm 0 \cdot 02$	$8 \cdot 620 \pm 0 \cdot 006$	$2 \cdot 3 \pm 0 \cdot 2$	$0 \cdot 35 \pm 0 \cdot 02$	$0 \cdot 15 \pm 0 \cdot 01$
Simple cubic	$1 \cdot 5 \pm 0 \cdot 1$	$10 \cdot 63 \pm 0 \cdot 05$	$2 \cdot 5 \pm 1 \cdot 0$	$0 \cdot 7 \pm 0 \cdot 2$	$0 \cdot 16 \pm 0 \cdot 03$
Body-centred cubic	$1 \cdot 55 \pm 0 \cdot 1$	$15 \cdot 3 \pm 0 \cdot 1$	$2 \cdot 4 \pm 1 \cdot 0$	$0 \cdot 6 \pm 0 \cdot 2$	$0 \cdot 11 \pm 0 \cdot 02$
Face-centred cubic	$1 \cdot 6 \pm 0 \cdot 1$	$23 \cdot 9 \pm 0 \cdot 1$	$> 2 \cdot 2$	$< 0 \cdot 7$	$0 \cdot 07 \pm 0 \cdot 02$

Looking at the individual entries, we see that for both the triangular site and bond problems, τ is very close to unity. If τ were precisely unity, the generating function would have a logarithmic divergence. For the square lattice site and bond problems, τ is again close to unity, though the uncertainty is respectively twenty and five times as great. Nevertheless, the results do suggest that in two dimensions $\tau = 1$ for both the site and the bond problems is likely to be a very good approximation.

For the three-dimensional lattices, the exponent estimates are less precise. There is a slight trend for τ to increase with lattice coordination number, and this possibility should be borne in mind. Nevertheless, taking into account the results obtained in two dimensions, a simpler and more appealing conclusion is that τ is the same for both bond and site problems for all lattices in three dimensions, and with a value of $1 \cdot 5$ or perhaps slightly higher. A value of $1 \cdot 5$ would correspond to a square root cusp in the generating function.

For all the lattices studied, for both the bond and site problems, the value of λ agrees with that obtained by Sykes *et al* to within numerical uncertainties. λ is seen to be lattice and model dependent, and for all lattices we have studied $\lambda_{site} < \lambda_{bond}$ (Whittington and Gaunt 1978). The ratio $\lambda_{site}/\lambda_{bond}$ appears to decrease with increasing coordination number.

The amplitude A is also seen to be lattice and model dependent, A decreasing with increasing coordination number, and it seems that $A_{site} > A_{bond}$ for each lattice.

Unfortunately we can say very little about F and θ. They are closely linked in the assumed functional form, in that a small change in one produces a large change in the other, without substantially changing the other three parameters A, λ and τ. We subsequently discuss this point further.

Another global trend is that the series behave better the higher the coordination number of the lattice. For this reason we have shown no results at this stage for the honeycomb and diamond lattices. This trend is also observed for other lattice models, such as the Ising and self-avoiding random walk models, but there it is clearer why the

topology of the more loose-packed lattices should affect the behaviour of the coefficients.

Paralleling the more conventional methods of series analysis, we sought to develop biased estimates of the parameters. Thus by fixing the value of the exponent τ to that previously obtained, namely $\tau = 1 \cdot 0$ in two dimensions, $\tau = 1 \cdot 5$ in three dimensions, a high degree of regularity was observed in the sequences for the other parameters.

Thus in two dimensions we observed that with τ fixed at $1 \cdot 0$, all the other parameters could be extrapolated with an apparently high degree of accuracy. Our results for the two-dimensional lattices so studied are shown in table 4 for both the bond and site problems. It is clear from these results that estimates of λ can be made very precisely, while estimates of the other parameters are less certain. A value of θ around $2 \cdot 2$ encompasses all the bond animal results, while for the site animals a lower value of around $1 \cdot 8$ seems more appropriate. Such values are consistent with the estimates in tables 2 and 3. The uncertainties are however too great for us to speculate on any lattice dependence of this parameter, though it appears that $\theta(\text{bond}) > \theta(\text{site})$, though even this can by no means be confidently asserted. The amplitude A is clearly lattice and model dependent as observed in tables 3 and 4 also. No clear trend is discernable from the estimates of F.

Table 4. Results of a four parameter fit to two-dimensional bond and site animals assuming $\tau = 1$.

Lattice	λ	θ	F	A
Honeycomb (bond)	$3 \cdot 367 \pm 0 \cdot 002$	$2 \cdot 1 \pm 0 \cdot 5$	$\simeq 0 \cdot 2$	$0 \cdot 40 \pm 0 \cdot 01$
Square (bond)	$5 \cdot 208 \pm 0 \cdot 004$	$2 \cdot 1 \pm 0 \cdot 3$	$0 \cdot 3 \pm 0 \cdot 1$	$0 \cdot 26 \pm 0 \cdot 02$
Triangular (bond)	$8 \cdot 620 \pm 0 \cdot 002$	$2 \cdot 33 \pm 0 \cdot 05$	$0 \cdot 33 \pm 0 \cdot 02$	$0 \cdot 154 \pm 0 \cdot 001$
Square (site)	$4 \cdot 063 \pm 0 \cdot 002$	$2 \cdot 0 \pm 0 \cdot 2$	$0 \cdot 5 \pm 0 \cdot 1$	$0 \cdot 31 \pm 0 \cdot 01$
Triangular (site)	$5 \cdot 183 \pm 0 \cdot 001$	$1 \cdot 75 \pm 0 \cdot 1$	$0 \cdot 348 \pm 0 \cdot 005$	$0 \cdot 275 \pm 0 \cdot 002$

Turning now to the series for the three-dimensional lattices we performed a similar analysis, with τ fixed at $1 \cdot 5$. We found that this produced much more regular sequences of estimates for all parameters, but that in most cases the sequences were increasing or decreasing in such a manner as to make extrapolation difficult. We found that a slight change in τ usually made the sequences much steadier, and more obviously extrapolable. This suggested a regularity criterion, whereby τ is varied until the most stable sequences for the other critical parameters are obtained. Proceeding in this way we obtained the results shown in table 5. It can be seen that values of τ ranging from $1 \cdot 50$ to $1 \cdot 58$ were found. This immediately suggests the possibility that τ is lattice dependent. There is no evidence of such lattice dependence in two dimensions, or in other lattice models, so we consider it most likely that it is an artifact of the method of analysis. Nevertheless, the possibility of lattice dependence should be borne in mind.

The estimates of λ agree, within quoted errors, with those of Sykes and Glen (1976) and Sykes *et al* (1976), though our confidence limits are rather narrower, in one case twenty times smaller. However, these confidence limits depend on the value of τ. If τ were slightly in error there would be a corresponding error in λ. As a rule of thumb, we find that a 1% increase in τ produces a $0 \cdot 02\%$ increase in λ.

Table 5. Results of a four parameter fit to three-dimensional bond and site animals. τ is chosen to regularise the other parameters.

Lattice	τ	λ	θ	F	A
Diamond (site)	1·55	5·55 ± 0·01	2·4 ± 0·4	2·5 ⊙ 0·5	0·29 ± 0·02
Simple cubic (site)	1·50	8·34 ± 0·02	2·0 ± 0·3	0·55 ± 0·25	0·19 ± 0·02
Body-centred cubic (site)	1·53	11·18 ± 0·01	1·6 ± 0·5	0·73 ± 0·06	0·16 ± 0·02
Face-centred cubic (site)	1·53	13·94 ± 0·01	1·65 ± 0·2	0·65 ± 0·1	0·14 ± 0·02
Diamond (bond)	1·55	6·130 ± 0·006	2·0 ± 0·1	0·65 ± 0·05	0·32 ± 0·01
Simple cubic (bond)	1·55	10·629 ± 0·006	2·25 ± 0·15	0·70 ± 0·05	0·172 ± 0·002
Body-centred cubic (bond)	1·58	15·302 ± 0·006	2·20 ± 0·1	0·70 ± 0·05	0·120 ± 0·002
Face-centred cubic (bond)	1·58	23·915 ± 0·01	2·3 ± 0·2	0·73 ± 0·04	0·077 ± 0·002

For the bond problem, we find θ is stable at around 2·2, while for the site problem θ is less stable, but for all but one lattice the central value is less than or equal to 2·0. Thus the observation that θ(bond) > θ(site) suggested by the results for two-dimensional animals also appears to hold for the three-dimensional animals. Both in two and three dimensions we find that $\theta = 2\cdot2$(bond) and $\theta = 1\cdot8$(site) encompass substantially all the results. There is therefore no *observed* dimensional dependence of θ. Our estimates of θ are however insufficiently precise to assert this confidently. For the three-dimensional bond problem, F is approximately constant at 0·7; however, the three-dimensional site problem estimates of F are too scattered for any trend to be discernible. For the amplitudes A we observe that A decreases with increasing coordination number, that A(site)/A(bond) = r, where $r > 1$ for all but the diamond lattice (where the uncertainties are largest) and increases with increasing coordination number.

In conclusion, we find that the asymptotic form proposed by Domb appears to fit the available data rather better than the simpler form assumed in previous analyses.

Acknowledgments

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