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A Monte Carlo study of lattice trails

A J Guttmann† and T R Osborn‡

† Department of Mathematics, University of Melbourne, Parkville, Victoria 3052, Australia
‡ School of Computing Sciences, NSWIT, PO Box 123, Broadway, NSW 2007, Australia

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Abstract. We use the recently developed Monte Carlo algorithm of Berretti and Sokal to study the critical behaviour of lattice trails on the square and triangular lattices. We find support for the earlier belief that this problem is in the same universality class as self-avoiding walks. Accepting this, we obtain the most precise estimates to date of the connective constants. It is argued that this problem is particularly well suited to study by Monte Carlo methods rather than by series analysis.

1. Introduction

In two earlier papers (Guttmann 1985a, b, hereafter referred to as I and II) an extensive analytic and numerical study of the configurational properties of lattice trails was made. Lattice trails bear the same relationship to self-avoiding walks as does the problem of bond percolation to the problem of site percolation. For a SAW we are interested in enumerating all connected paths such that no site is visited more than once (this of course also precludes multiple bond occupancy). For the problem of lattice trails, the problem is to enumerate all connected paths such that no bond is revisited, but sites may be revisited.

In I we proved that the trails problem is in the same universality class as the SAW problem for the two-dimensional hexagonal lattice and the three-dimensional Lave lattice, but no proof has been found for lattices of a higher coordination number. Nevertheless, we argued in I and II that an extensive body of numerical evidence indicated that this was also the case for the other regular two- and three-dimensional lattices. However, despite the availability of quite long series expansions for the trail generating function, the results of this analysis were comparatively disappointing, insofar as they indicated a critical exponent γ of the trail generating function of around 1.40, compared to the SAW value of $\gamma = 1.343\ 75$.

This was ascribed to the presence of non-physical singularities quite close to the circle of convergence of the generating function, complicated by a more intrusive confluent singularity structure than that prevailing for SAW.

For the mean square end-to-end distance exponent ν the situation was better. In II we studied the difference $\nu_{\mathrm{saw}} - \nu_{\mathrm{trails}}$ and found this to be indistinguishable from 0 for the square lattice. Subsequently, Rapaport (1985) also studied the trails problem, both by series expansion methods (for the three-dimensional FCC lattice) and by Monte Carlo methods in order to estimate ν. His results were entirely consistent with those found in the earlier study discussed.

In this paper we use the appropriate modified Berretti-Sokal (1985, hereafter referred to as BS) Monte Carlo algorithm to study the trails problem on the square and triangular lattices. We only sketch the method here. It is a dynamic MC algorithm, generating trails in the grand canonical ensemble

$$\text{Prob}(\text{length} = N) = \text{constant} \times \beta^N t_N \tag{1}$$

where t_N is the number of distinct N-step trails, and β is a user-chosen parameter which determines the expectation value of the length of the trails. The algorithm starts with the empty trail, and each step of the algorithm consists either of appending a step to the end of the walk (randomly in one of the q lattice directions), or else deleting the last step. In the former case, the step is allowed if the resultant path is a trail. The relative probabilities of these two types of moves are chosen so as to satisfy detailed balance for the measure (1). These conditions allow a trail of arbitrary length to evolve to or from the initial configuration (the empty trail), as is clearly necessary for the ergodicity of the algorithm.

The trails are assumed to have the asymptotic behaviour

$$t_N = A\lambda^N N^{\gamma-1}(1 + a/N + \ldots) \tag{2}$$

for large N, and we use the maximum likelihood estimation (MLE) of BS to determine the connective constant λ and the critical exponent γ. The autocorrelation time of the algorithm, τ, is of order $\langle N\rangle^2$ and is estimated numerically using standard methods of statistical time series analysis, as elucidated by BS.

The parameter β is related to the average trail size by

$$\langle N\rangle \approx \beta\lambda\gamma/(1-\beta\lambda). \tag{3}$$

As there is little doubt that the model is in the same universality class as SAW, our main purpose was to see if Monte Carlo methods, which enable us to study longer walks than those available by series expansions, would produce more accurate estimates of the connective constant λ, and also shed some light on why the series expansions for the trails problem behave substantially worse than those for the SAW problem.

2. Data generation and analysis

For both the square and triangular lattices we generated a sample of 10^9 Monte Carlo iterations. Each of the two data sets took approximately 50 h CPU time on a Perkin Elmer 3220 minicomputer. For the square lattice data the run was performed with $\beta = 0.365$, corresponding to $\langle N\rangle = 191$, while for the triangular lattice the run was performed with $\beta = 0.2195$, corresponding to $\langle N\rangle = 199$. Data were taken once every 10^5 MC iterations, and in doing the statistical analysis we skipped the data from the first 10^8 iterations; since this is some 500 times the algorithm's autocorrelation time (given below), there should be no doubt that equilibrium has been reached. Details of the random number generator used are given in Guttmann *et al* (1986).

An autocorrelation analysis gave $\tau = 200\,000$ MC iterations, so that $\tau = 5\langle N\rangle^2$, as for SAW (see BS, Guttmann *et al* 1986).

Following our analysis for the SAW case, we first performed a maximum-likelihood estimation of γ and λ, using the ansatz

$$t_N = \lambda^N (N+3)^{\gamma-1} A[1 + a_1/(N+3)] \qquad \text{for } N > N_{\min} \tag{4}$$

for a range of values of a_1 and N_{min}; the results, for the triangular lattice, are shown in table 1. The errors shown are 95% confidence intervals, and represent statistical errors only. A corresponding table for SAW is given in Guttmann *et al* (1986). As in that case, for $N_{min} = 0$, the estimates are biased by strong systematic error due to corrections to scaling not included in (4), while as N_{min} increases, so does the statistical error, as the sample size clearly decreases with increasing N_{min}.

Following BS, we attempt to invoke their 'flatness criterion' in order to find a region for which the 'true' values of λ and γ are included. This turns out to be quite difficult—again paralleling the SAW case—and we are forced to include all values of a_1 in the range $-0.5 < a_1 < 0.75$ and $20 < N_{min} < 80$. For $N = 120$ the statistical errors are already too large. In this way we arrive at conservative estimates for both λ and γ, by using all bold entries in table 1, and so obtain

$$\begin{aligned} \lambda &= 4.5258 \pm 0.0016 \pm 0.0015 \qquad \text{(triangular)} \\ \gamma &= 1.31 \pm 0.12 \pm 0.08 \end{aligned} \tag{5}$$

where the first errors represent systematic error due to unincluded corrections to scaling

Table 1. Two-parameter maximum-likelihood estimates of λ and γ, assuming (4). Error bars include statistical errors only, and represent 95% confidence limits.

	N						
a	0	20	40	80	120	160	200
−0.75	4.525 145	4.525 528	4.525 542	4.526 547	4.527 284	4.528 261	4.528 731
	0.001 020	0.001 243	0.001 458	0.001 876	0.002 349	0.002 876	0.003 502
	1.344 355	1.323 301	1.322 886	1.245 548	1.177 650	1.077 054	1.027 321
	0.039 101	0.057 205	0.076 908	0.121 722	0.178 953	0.250 524	0.342 247
−0.50	4.524 992	**4.525 485**	**4.525 515**	**4.526 533**	4.527 274	4.528 254	4.528 725
	0.001 020	**0.001 243**	**0.001 458**	**0.001 876**	0.002 349	0.002 876	0.003 502
	1.354 553	**1.327 411**	**1.325 860**	**1.247 606**	1.179 273	1.078 411	1.028 496
	0.039 001	**0.057 204**	**0.076 912**	**0.121 729**	0.178 959	0.250 531	0.342 255
−0.25	4.524 844	**4.525 442**	**4.525 489**	**4.526 519**	4.527 625	4.528 247	4.528 720
	0.001 020	**0.001 243**	**0.001 459**	**0.001 877**	0.002 350	0.002 876	0.003 502
	1.364 415	**1.331 486**	**1.328 817**	**1.249 656**	1.180 891	1.079 765	1.029 669
	0.038 908	**0.057 203**	**0.076 916**	**0.121 735**	0.178 966	0.250 539	0.342 263
0.00	4.524 702	**4.525 399**	**4.525 463**	**4.526 504**	4.527 255	4.528 240	4.528 714
	0.001 020	**0.001 244**	**0.001 459**	**0.001 877**	0.002 350	0.002 877	0.003 502
	1.373 963	**1.335 524**	**1.331 756**	**1.251 698**	1.182 505	1.081 117	1.030 839
	0.038 822	**0.057 202**	**0.076 919**	**0.121 741**	0.178 973	0.250 546	0.342 270
0.25	4.524 565	**4.525 357**	**4.525 437**	**4.526 490**	4.527 246	4.528 233	4.528 709
	0.001 020	**0.001 244**	**0.001 459**	**0.001 877**	0.002 350	0.002 877	0.003 502
	1.383 216	**1.339 528**	**1.334 679**	**1.253 733**	1.184 115	1.082 465	1.032 008
	0.038 741	**0.057 201**	**0.076 923**	**0.121 747**	0.178 980	0.250 553	0.342 278
0.50	4.524 433	**4.525 316**	**4.525 411**	**4.526 476**	4.527 236	4.528 226	4.528 704
	0.001 020	**0.001 245**	**0.001 459**	**0.001 877**	0.002 350	0.002 877	0.003 503
	1.392 194	**1.343 497**	**1.337 586**	**1.255 761**	1.185 721	1.083 810	1.033 173
	0.038 666	**0.057 201**	**0.076 927**	**0.121 753**	0.178 987	0.250 560	0.342 286
0.75	4.524 306	**4.525 274**	**4.525 386**	**4.526 462**	4.527 227	4.528 220	4.528 699
	0.001 020	**0.001 245**	**0.001 460**	**0.001 877**	0.002 350	0.002 877	0.003 503
	1.400 911	**1.347 431**	**1.340 475**	**1.257 781**	1.187 321	1.085 152	1.034 337
	0.038 595	**0.057 200**	**0.076 931**	**0.121 759**	0.178 993	0.250 568	0.342 293

(95% confidence limits—subjective) and the second error is statistical error taken at $N_{\min}=40$ (95% confidence limits).

For the square lattice data, a similar table (not shown) gave a wide spread of values for which the flatness criteria applied, $-0.5 < a_1 < 0.5$ and $20 < N_{\min} < 120$, and combining these gave the estimates

$$\begin{aligned} \lambda &= 2.7205 \pm 0.0007 \pm 0.0009 \qquad \text{(square)} \\ \gamma &= 1.348 \pm 0.099 \pm 0.0079. \end{aligned} \tag{6}$$

It might be argued that the ansatz (4) ignores non-analytic correction-to-scaling terms, which seem likely to be present in this problem. However, due to the large statistical errors, it is not possible to distinguish between a non-analytic and analytic correction to scaling term—indeed, any such correction is likely to be effectively represented by a change in a_1.

As in the SAW case, these results are consistent with Nienhuis' (1982, 1984) exact result $\gamma=\frac{43}{32}$, but with such wide error bars as to be of little interest. If we accept this result, however, and re-analyse our data with this value of γ fixed, we obtain rather better results.

In table 2 we show the results for the square lattice data, and use those shown in bold to which our, by now relatively unselective, flatness criterion applies. That is, we have chosen the same range of values as used above in the unbiased analysis. A similar analysis is applied to the triangular lattice data (not shown) and our results in the two cases are

$$\begin{aligned} \lambda &= 2.720\,59 \pm 0.000\,42 \pm 0.000\,37 \qquad \text{(square)} \\ \lambda &= 4.525\,26 \pm 0.000\,15 \pm 0.000\,65 \qquad \text{(triangular).} \end{aligned} \tag{7}$$

The estimates and error bars in tables 1 and 2 were computed by using all data as if they were independent, and then multiplying the MLE theory error bars by a factor $(2\tau)^{1/2}$ to adjust for the effects of autocorrelations. As shown in Guttmann *et al* (1986), alternative analyses seem to give indistinguishably close results.

Table 2. One-parameter maximum likelihood estimates of λ, assuming (4), with $\gamma=\frac{43}{32}$. Error bars include statistical errors only, and represent 95% confidence limits.

	N						
a	0	20	40	80	120	160	200
−0.75	2.720 734	2.720 656	2.720 579	2.720 590	2.720 516	2.720 473	2.720 526
	0.000 336	0.000 349	0.000 367	0.000 410	0.000 463	0.000 523	0.000 592
−0.50	2.720 779	**2.720 679**	**2.720 595**	**2.720 600**	**2.720 523**	2.720 478	2.720 530
	0.000 335	**0.000 349**	**0.000 367**	**0.000 410**	**0.000 463**	0.000 523	0.000 592
−0.25	2.720 825	**2.720 702**	**2.720 611**	**2.720 610**	**2.720 529**	2.720 483	2.720 534
	0.000 334	**0.000 349**	**0.000 367**	**0.000 410**	**0.000 462**	0.000 523	0.000 592
0.00	2.720 870	**2.720 724**	**2.720 627**	**2.720 620**	**2.720 536**	2.720 488	2.720 538
	0.000 3334	**0.000 348**	**0.000 367**	**0.000 410**	**0.000 462**	0.000 523	0.000 592
0.25	2.720 914	**2.720 747**	**2.720 643**	**2.720 629**	**2.720 543**	2.720 493	2.720 542
	0.000 333	**0.000 348**	**0.000 367**	**0.000 410**	**0.000 462**	0.000 523	0.000 592
0.50	2.720 958	**2.720 769**	**2.720 659**	**2.720 639**	**2.720 550**	2.720 498	2.720 546
	0.000 332	**0.000 348**	**0.000 366**	**0.000 410**	**0.000 462**	0.000 523	0.000 592
0.75	2.721 001	2.720 792	2.720 674	2.720 649	2.720 557	2.720 503	2.720 550
	0.000 332	0.000 347	0.000 366	0.000 410	0.000 462	0.000 523	0.000 592

3. Discussion

If we now compare these results with the series results obtained in II, we find satisfactory agreement. For the triangular lattice case the series estimate was $\lambda = 4.524 \pm 0.004$, while for the square lattice the series estimate was $\lambda = 2.7215 \pm 0.002$. It can be seen that the MC estimates are significantly more accurate than the series estimates in this case—in contrast to the SAW case—and allow us to rule out a conjecture of Malakis (1975) that $\lambda(\text{square}) = e = 2.718\,28\ldots$ at the 99.9% confidence level.

The trails problem is seen to be one in which Monte Carlo analysis does a better job than does series analysis, whereas for the SAW problem and perhaps for the Ising problem the opposite is the case. As noted in II, this is likely to be due to the presence of competing singularities, as well as the effect of more prominent correction-to-scaling terms. The effect of these on our ansatz (4) has already been discussed in Guttmann *et al* (1986). The upshot of these remarks though is that asymptotic behaviour has not yet set in at trail lengths of 14–22, which is the size of the maximum length trails accessible by series analysis. Thus this problem is a particularly appropriate one for MC algorithms to be tested against.

The trails problem was also studied by Zhou and Li (1984) using series analysis. Their conclusion, that the problem is in a distinct universality class from SAW, is not supported. Rather, it adds weight to our conclusion that this problem does not readily lend itself to study by series analysis, but that Monte Carlo methods are more appropriate.

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