

On the number of anisospiral walks: a challenge in numerical analysis

Aleksander L Owczarek & Andrew Rechnitzer

Department of Mathematics and Statistics & MASCOS,

The University of Melbourne, Parkville Victoria 3010, Australia.

email: A.Owczarek@ms.unimelb.edu.au & A.Rechnitzer@ms.unimelb.edu.au

Date submitted: . Date accepted: .

October 21, 2005

Abstract

The numerical analysis of combinatorial problems with non-standard scaling is an important testing ground for the limits of current techniques. One problem that has proven especially difficult to analyse with all available numerical techniques, including various Monte Carlo simulation methods and careful series analysis, is *anisotropic spiral walks* in two dimensions. Here we revisit this problem discussing various non-standard scaling hypotheses and showing how these best fit the available data. This highlights the difficulties with the analysis of data when the standard scaling forms may not hold true and also provides a testing ground for improved techniques.

1 Introduction

The scaling behaviour of thermodynamic, geometric and topological properties of long chain polymers in solution have been studied using many different models in statistical mechanics. One large group of such models are lattice based and involve *self-avoiding walks* (SAWs) and their derivatives.

A large number of modifications have been made to the basic SAW model to mimic different physical situations or to make the model easier to analyse and (in some cases) solve. Some of these modifications (such as directedness) change the scaling behaviour of system properties and so change the universality class of the model.

For example, restricting the model by only allowing steps in the positive axial directions, and so producing a fully directed walk model changes the scaling of the metric properties of the system. The fully directed walk model just described is an example of a *two-step restricted walk*.

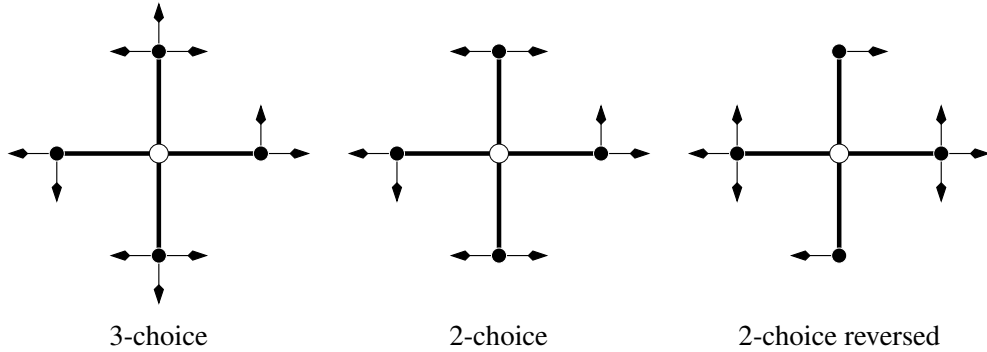


Figure 1: The three-choice and two-choice stepping rules. Also shown is the “reverse” of the two-choice rule. The reverse of the three-choice rule is itself.

A two-step restricted walk (TSRW) is a self-avoiding walk for which only certain pairs of steps are allowed — *e.g.* after an east step the walk may only step north or east. Guttmann *et al.* [3] surveyed the universality classes of TSRWs on the square lattice and attempted to establish a link between the universality classes and the symmetry properties of the underlying rules. A subsequent survey in three dimensions concluded that the only non-directed or non-trivial universality class is that of self-avoiding walks [9].

In two dimensions it is thought [3, 9, 8] that TSRWs fall into the following universality classes (according to their metric exponents): self-avoiding walks, spiral walks, anisotropic spiral walks, directed walks, one-dimensional walks, trivial or zero-dimensional walks. The scaling of entropic and metric properties of walks in each of these classes, *except* anisotropic spiral walks, is well understood.

In this paper we return again to the analysis of walks in the anisospiral universality class: three-choice and two-choice walks. The rules for these walks are given in Figure 1. The “two-choice reversed” rule is the two-step rule for a two-choice walk with its orientation reversed. The “three-choice reverse” rule is simply another three-choice rule.

These models were introduced by Manna [7] in 1984 and he analysed the following scaling form

$$c_n \sim A\mu^n n^g, \quad (1)$$

which led him to propose that these models do not lie in either the SAW or spiral walk universality classes. Shortly afterwards Whittington [12] proved that

$$\mu = \lim_{n \rightarrow \infty} c_n^{1/n} = \begin{cases} (1 + \sqrt{5})/2 & \text{for two-choice walks,} \\ 2 & \text{for three-choice walks.} \end{cases} \quad (2)$$

A careful analysis of series data [4] suggested the following scaling form for the number of walks of length n

$$c_n \sim A\mu^n \exp(\beta n^{1/2}) n^g, \quad (3)$$

which is a mixture of the SAW and spiral walk scaling forms. Unfortunately the data was poorly behaved and fitting was extremely difficult; they obtained the following estimates of

β and g :

$$\beta = \begin{cases} 0.13(3) & \text{two-choice} \\ 0.15(3) & \text{three-choice} \end{cases} \quad g = \begin{cases} -0.8(2) & \text{two-choice} \\ -0.9(2) & \text{three-choice} \end{cases} \quad (4)$$

The metric properties of these models have also been studied. Series analysis [7, 3] demonstrated that the walks scale anisotropically and form a new universality class. Later Monte Carlo work gave substantially different exponent estimates providing compelling evidence that the models suffer from strong corrections to scaling.

We point out that usually in the study of walk models, the open walk model and the closed walk, or polygon, model behave in a related manner: the form of the asymptotic scaling of model quantities is the same. For three-choice anisospiral walks this is not the case. The polygon model is a lot simpler since no spiral configurations, the dominant contribution to the walk partition sum, can occur. In fact, the polygon model is now exactly solved [2].

Rather than studying the metric properties of these models, in this work we examine the scaling of the number of these walks using a combination of the inhomogeneous pivot algorithm [1] and the method of atmospheres [10, 11]. This allows us to test the validity of various possible scaling forms. These techniques are described in the next section. In Section 3 we analyse our data and use it to study different scaling forms for c_n .

2 Scaling and Monte Carlo

2.1 The inhomogeneous pivot algorithm

One of the most efficient (if not the most efficient) canonical algorithm for sampling self-avoiding walks is the pivot algorithm [5, 6]. This algorithm cannot be directly applied to two-choice and three-choice walks. Instead we apply the *inhomogeneous pivot* algorithm developed by Brak, Owczarek and Soteros in [1].

The algorithm augments the standard non-local pivot moves with a local move that changes the orientation of a single step. When a pivot or local move is chosen, the resulting configuration is only accepted if it is both self-avoiding and still obeys the two-step rule — *i.e.* the resulting walk is still two-choice or three-choice.

Though this algorithm is a canonical algorithm, we are able to use it in conjunction with the method of atmospheres to investigate the scaling behaviour of the number of walks.

2.2 Method of atmospheres

Even though the pivot algorithm is a canonical (fixed-length) algorithm, we are still able to use it to study the c_n . Unfortunately we are not able to obtain direct estimates of c_n , however, the method of atmospheres [10, 11] allows us to study c_n indirectly, in that it gives estimates of ratios c_{n+k}/c_n for fixed k .

Let φ be a walk of length n . Let $a_k(\varphi)$ be the set of all walks which reduce to φ when their last k steps are removed. Alternatively $a_k(\varphi)$ is the set of all walks obtained from φ by adding k steps to its end. We call $|a_k(\varphi)|$ the k^{th} *atmosphere* of φ .

The sum over all walks of length n of the k^{th} atmosphere is simply the number of walks of length $n+k$. Hence, the mean k^{th} atmosphere across all walks of length n is equal to

$$\langle \text{atm}_k \rangle_n = \frac{1}{c_n} \sum_{|\varphi|=n} |a_k(\varphi)| = \frac{c_{n+k}}{c_n} \quad (5)$$

Using the inhomogeneous pivot algorithm we can estimate mean atmospheres and hence the ratios c_{n+k}/c_n for two-choice and three-choice walks.

While these estimates do not allow us *direct* access to the scaling of c_n , they do provide us with a means of testing the validity of different scaling forms. For example, if the number of walks scales as a simple exponential (*i.e.* the dominant singularity of the generating function is a simple pole) then

$$c_n \sim A\mu^n \quad \implies \quad \frac{c_{n+k}}{c_n} \sim \mu^k \approx \text{a constant} \quad (6)$$

3 Analysis of atmospheres

We used the inhomogeneous pivot algorithm to sample both two-choice and three-choice walks uniformly at random. For each sampled walk we computed the first 6 atmospheres using a simple back-tracking algorithm. The mean atmospheres were then computed and the corresponding errors were estimated using auto-correlation times (using code provided to us by Prof. Buks van Rensburg). We found that the relative error in our estimates of the k^{th} atmosphere became substantially smaller with increasing k . Hence we generally analysed the mean sixth atmosphere and then confirmed our results using the other quantities.

We first made precise estimates of the mean first through sixth atmospheres for both two-choice and three-choice walks for short lengths. These estimates were not used in the subsequent analysis but instead allowed us to check the technique against exact enumeration data. We then estimated the mean first through sixth atmospheres for a range of lengths between 100 and 2000 steps. These were then used to assess the validity of different scaling hypotheses.

In previous work, Manna [7] and Guttmann and Wallace [4] have investigated two different scaling forms for c_n . These two forms imply the following scaling forms for the mean atmosphere:

$$c_n \sim A\mu^n n^g \quad \implies \quad \frac{c_{n+k}}{c_n} \sim \mu^k \left(1 + \frac{kg}{n} + \frac{k^2 g(g-1)}{2n^2} + O(n^{-3}) \right), \quad (7)$$

$$c_n \sim A\mu^n \exp(\beta\sqrt{n}) n^g \quad \implies \quad \frac{c_{n+k}}{c_n} \sim \mu^k \left(1 + \frac{k\beta}{2\sqrt{n}} + \frac{k^2\beta^2 + 8kg}{8n} + O(n^{-3/2}) \right). \quad (8)$$

In Figure 2 we plot the mean sixth atmosphere against $1/n$ and $1/\sqrt{n}$. Plots of the same quantity for three-choice walks are very similar. Indeed all of these plots display considerable curvature; this indicates that either that the sub-dominant terms in equations (7) and (8) are still quite strong or that forms are not valid.

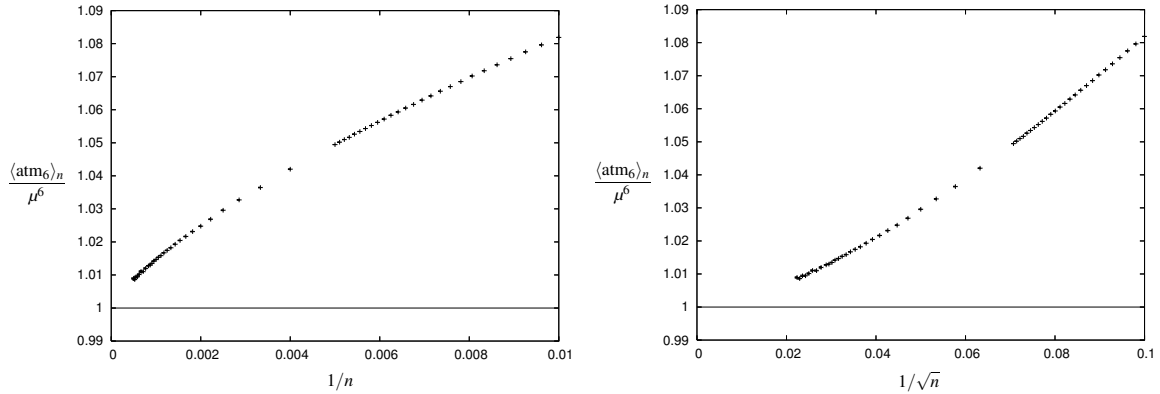


Figure 2: Plots of $\langle \text{atm}_6 \rangle_n \mu^{-6}$ against $1/n$ (left) and $1/\sqrt{n}$ (right) with $\mu = (1 + \sqrt{5})/2$. The error bars on these points are approximately the size of the symbols. The plots of the mean first through fifth atmospheres are very similar. Both plots show that this quantity is converging to 1, but also show considerable curvature.

Simple linear fits of our data (for lengths 100 to 2000) to equation (7), using the exact values of μ , give the following estimates of g

$$g \approx \begin{cases} 2.1 & \text{two-choice} \\ 2.4 & \text{three-choice} \end{cases} \quad (9)$$

However the estimates of the $O(n^{-2})$ correction term were not of the form $\frac{k^2 g(g-1)}{2}$ — indeed they were quite large, negative and roughly proportional to k rather than k^2 .

Similar fits of our data (for lengths 100 to 2000) to equation (8) give the following estimates of β and g :

$$\beta \approx \begin{cases} 0.05 & \text{two-choice} \\ 0.06 & \text{three-choice} \end{cases} \quad g \approx \begin{cases} 0.9 & \text{two-choice} \\ 1.0 & \text{three-choice} \end{cases} \quad (10)$$

We note immediately that these estimates of β are substantially less than those obtained from series analysis (equation (4)) while the estimates of g are likewise larger. Additionally, fitting our data from length 100 to N_{max} we found that as N_{max} increased, the estimate of β slowly decreased while the estimate of g increased. This strongly suggests that the scaling form is not correct.

Since our data does not strongly support either of the above two scaling forms, we decided to examine the more general form:

$$c_n \sim A\mu^n \exp(\beta n^\delta) n^g. \quad (11)$$

with $0 < \delta < 1$. This implies the following scaling form for the k^{th} atmosphere

$$\frac{c_{n+k}}{c_n} \sim \mu^k \left(1 + \delta \frac{k\beta}{n^{1-\delta}} + \delta^2 \frac{k^2 \beta^2}{2n^{2-2\delta}} + O(n^{-2+\delta}) \right) \cdot \left(1 + \frac{kg}{n} + O(n^{-2}) \right). \quad (12)$$

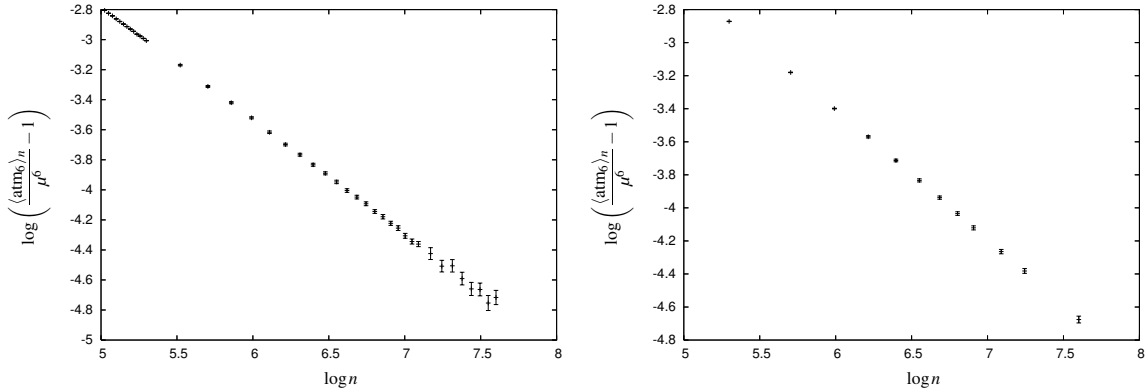


Figure 3: Plots of $\log \left(\frac{\langle \text{atm}_k \rangle_n}{\mu^k} - 1 \right)$ against $\log n$ for both two-choice (left) and three-choice (right) walks.

Since the value of μ is known for both models, we are able to estimate δ using

$$\log \left(\frac{\langle \text{atm}_k \rangle_n}{\mu^k} - 1 \right) \sim (\delta - 1) \log n + \log(\delta k \beta) + \frac{g}{\delta b n^\delta} + o(n^{-\delta}). \quad (13)$$

While the presence of the $n^{-\delta}$ term means that we cannot use linear regression, plots of this quantity for both two-choice and three-choice walks (see Figure 3) show that it is very nearly linear in $\log n$. This linearity suggests that the $o(1)$ terms are very small, and so if we disregard these terms and fit against

$$\log \left(\frac{\langle \text{atm}_k \rangle_n}{\mu^k} - 1 \right) \sim (\delta - 1) \log n + \log(\delta k \beta) + o(1) \quad (14)$$

we obtain the following estimates of δ and β :

$$\delta = \begin{cases} 0.25(2) & \text{two-choice} \\ 0.22(2) & \text{three-choice} \end{cases} \quad \beta = \begin{cases} 1.9(2) & \text{two-choice} \\ 2.5(2) & \text{three-choice} \end{cases} \quad (15)$$

The mean first through sixth atmospheres all gave quite consistent estimates of these two numbers.

While the above values are close to the appealing values of $1/4$, $2/9$ or $1/5$, a closer examination of the data suggests that the $n^{-\delta}$ corrections in equation (13) are not completely negligible and so the above error bars should be treated with caution. Estimating δ using data from lengths 100 to N_{max} shows that δ decreases slowly as N_{max} is increased. Unfortunately fixing the value of δ (to say $2/9$ or $1/5$) and then fitting to equation (12) or (13) does not give meaningful results since the estimates of β and g are very sensitive to changes in δ .

In summary, we conclude that our data does not support either of the scaling forms studied previously (equations (1) and (3)). Rather we find evidence for equation (11) with a value of $\delta \approx 0.2 \sim 0.25$. Unfortunately we have not been able to obtain good estimates of the parameters β and g in this scaling form due to the sensitivity of estimates to errors in δ . We are *not* concluding that the scaling form (11) is indeed correct, just that, even without

the n^g factor, it is far more plausible numerically than the standard forms. This highlights the difficulty in analysing statistical mechanical models numerically where scaling forms are uncertain (such numerical problems are well known to statisticians). However, it conversely provides an opportunity to test any upgraded versions of numerical techniques, including both series analysis and Monte Carlo. We hope these models provide the inspiration for such improved techniques.

Acknowledgements

Financial support from the Australian Research Council and the Centre of Excellence for Mathematics and Statistics of Complex Systems is gratefully acknowledged by the authors. The authors also thank Tony Guttmann for suggesting these models to us originally, and hope that one day he can take these problems back again.

References

- [1] R. Brak, A. L. Owczarek, and C. E. Soteris. On anisotropic spiral self-avoiding walks. *J. Phys. A: Math. Gen.*, 31:4851–4869, 1998.
- [2] A. J. Guttmann and I. Jensen. math.CO/0506317, (2005).
- [3] A. J. Guttmann, T. Prellberg, and A. L. Owczarek. On the symmetry classes of planar self avoiding walks. *J. Phys. A: Math. Gen.*, 26:6615–6623, 1993.
- [4] A. J. Guttmann and K. J. Wallace. Two-dimensional spiral self-avoiding walks. *J. Phys. A: Math. Gen.*, 19:1645–1653, 1986.
- [5] M. Lal. Monte carlo computer simulation of chain molecules I. *Mol. Phys.*, 17:57–64, 1969.
- [6] N. Madras and G. Slade. *The Self-Avoiding Walk*. Birkhäuser, Boston, 1993.
- [7] S. S. Manna. Critical behaviour of anisotropic spiral self avoiding walks. *J. Phys. A: Math. Gen.*, 17:L899–L903, 1984.
- [8] A. L. Owczarek, A. Rechnitzer, and L. H. Wong. Addendum to “On three-dimensional self-avoiding walk symmetry classes”. *J. Phys. A: Math. Gen.*, 34:6055–6060, 2001.
- [9] A. Rechnitzer and A. L. Owczarek. On three-dimensional self-avoiding walk symmetry classes. *J. Phys. A: Math. Gen.*, 33:2685–2723, 2000.
- [10] A. Rechnitzer and E. J. Janse van Rensburg. Canonical monte carlo determination of the connective constant of self-avoiding walks. *J. Phys. A: Math. Gen.*, 35:L605–L612, 2002.

- [11] E. J. Janse van Rensburg and A. Rechnitzer. High precision canonical monte carlo determination of the growth constant of square lattice trees. *Phys. Rev. E*, 67:036116, 2003.
- [12] S. G. Whittington. The asymptotic form for the number of spiral self-avoiding walks. *J. Phys. A: Math. Gen.*, 17:L117–L119, 1984.