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## FAST TRACK COMMUNICATION

# Generalized atmospheric Rosenbluth methods (GARM)

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Online at [stacks.iop.org/JPhysA/41/442002](http://stacks.iop.org/JPhysA/41/442002)**Abstract**

We show that the classical Rosenbluth method for sampling self-avoiding walks (Hammersley and Morton 1954 *J. R. Stat. Soc. B* **16** 23, Rosenbluth and Rosenbluth 1955 *J. Chem. Phys.* **23** 356) can be extended to a general algorithm for sampling many families of objects, including self-avoiding polygons. The implementation relies on an elementary move which is a generalization of kinetic growth; rather than only appending edges to the endpoint, edges may be inserted at any vertex provided the resulting objects still lie within the same family. This gives, for the first time, a kinetic growth algorithm for sampling self-avoiding polygons. We implement this method using pruning and enrichment (Grassberger 1997 *Phys. Rev. E* **56** 3682) to sample self-avoiding walks and polygons. The algorithm can be further extended by mixing it with length-preserving moves, such as pivots and crank-shaft moves.

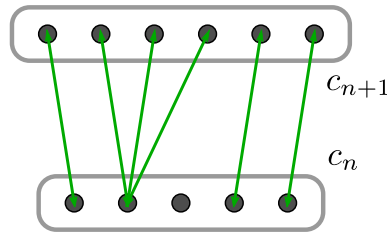
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(Some figures in this article are in colour only in the electronic version)

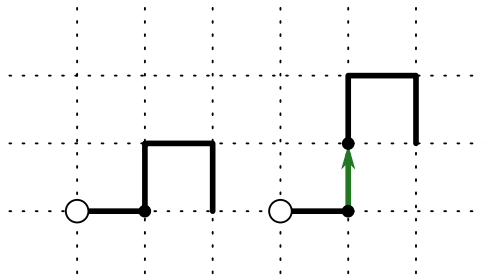
Monte Carlo simulations of self-avoiding walks (SAWs) and self-avoiding polygons (SAPs) on regular lattices are a major tool for the study of polymer statistics [4]. While kinetic growth algorithms [1, 2] have been used to sample SAWs to great success, it is unclear how they might be applied to SAPs. SAPs are models of ring polymers, plasmids (mitochondrial DNA) [5–7] and appear in the zero-component limit of the  $N$ -vector model [8]. In this paper, we generalize a growth algorithm for SAWs and show how it may be used to sample SAPs and other objects.

The Rosenbluth method for sampling self-avoiding walks (SAWs) is a classical algorithm dating back to the 1950s [1, 2]. This method found a new application with the development of a pruned and enriched implementation, called PERM, due to Grassberger [3]. This was in turn further extended using flat-histogram and multicanonical methods [9, 10]. These new algorithms have found many applications in the modelling of polymers (e.g. [11–13]).





**Figure 2.** A schematic picture of the linkages between  $c_n$  and  $c_{n+1}$ . There is one conformation with empty positive atmosphere.



**Figure 3.** The SAW on the right is obtained from the SAW on the left by inserting a north edge at the black vertex. This is one of its eleven positive atmospheric edges. It has three negative atmospheric edges.

Appending a positive atmospheric edge to  $\omega$  to obtain  $\omega'$  creates a linkage  $(\omega, \omega')$  (see figure 2). Deleting the last edge from  $\omega'$  gives  $\omega$ ; we define the *negative endpoint atmosphere* of  $\omega'$  to be this edge. We denote the size of the negative endpoint atmosphere of  $\omega'$  by  $a_-^e(\omega')$  and we again abuse notation by also using this symbol to denote the set of such edges. In the present context  $a_-^e(\omega') \equiv 1$ , but below we consider more general positive and negative atmospheres (which we will denote by ' $a_{\pm}(\omega)$ ' without the 'e' superscript).

By counting the number of linkages, we see that

$$\text{number of linkages} = \sum_{\omega} a_+^e(\omega) = \sum_{\omega'} a_-^e(\omega') = c_{n+1}. \tag{3}$$

This implies that

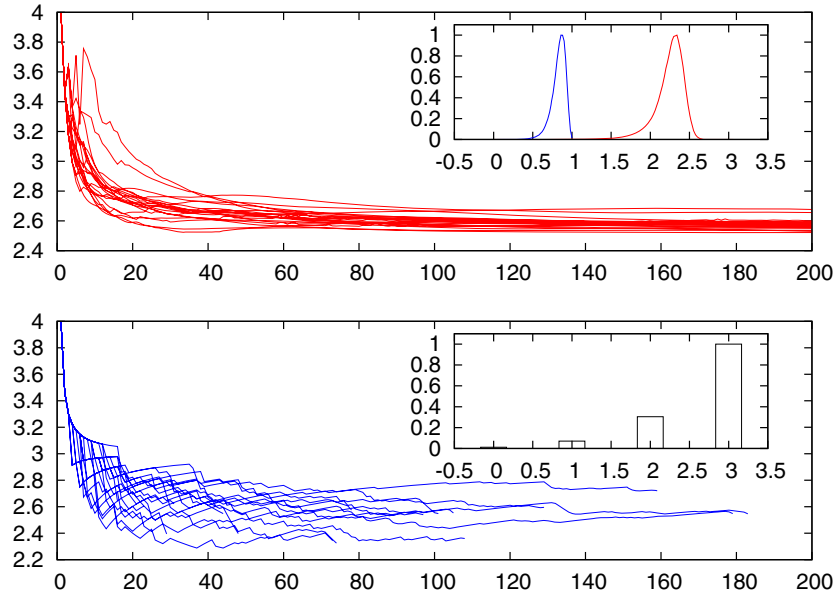
$$\frac{\langle a_+^e \rangle_n}{\langle a_-^e \rangle_{n+1}} = \frac{c_{n+1}}{c_n}, \tag{4}$$

where  $a_-^e(\omega') \equiv 1$  and the averages are taken over the uniform distribution.

This observation can be used to estimate growth constants and free energies of SAWs and bond trees [14–16]. We extend these definitions and show how they lead to a significant generalization of the Rosenbluth algorithm.

Define the positive atmosphere,  $a_+(\omega)$ , to be the number of ways that an edge can be inserted into  $\omega$  at any of its vertices so that a SAW is obtained (see figure 3). Note that there are SAWs with empty positive atmosphere.

Inserting a positive atmospheric edge into  $\omega$  results in a new SAW,  $\omega'$ . The negative atmosphere,  $a_-(\omega')$ , is the number of ways that an edge can be deleted to obtain a SAW.



**Figure 4.** Typical evolution of  $W(\varphi)^{1/n}$  against length for both GARM sampling (top) and Rosenbluth sampling (bottom). Shown are 20 samples from each. While GARM does suffer from attrition, SAWs sampled by Rosenbluth have larger variance and a higher rate of attrition. The insets show the distributions of positive and negative atmospheres per vertex (top) and endpoint atmospheres (bottom); the peak heights have been normalized to 1.

Linkages are created as above and by similar arguments to those leading to equation (4) we find

$$\frac{\langle a_+ \rangle_n}{\langle a_- \rangle_{n+1}} = \frac{c_{n+1}}{c_n}. \tag{5}$$

Simulations show that the distribution of atmospheres is narrowly peaked (see figure 4).

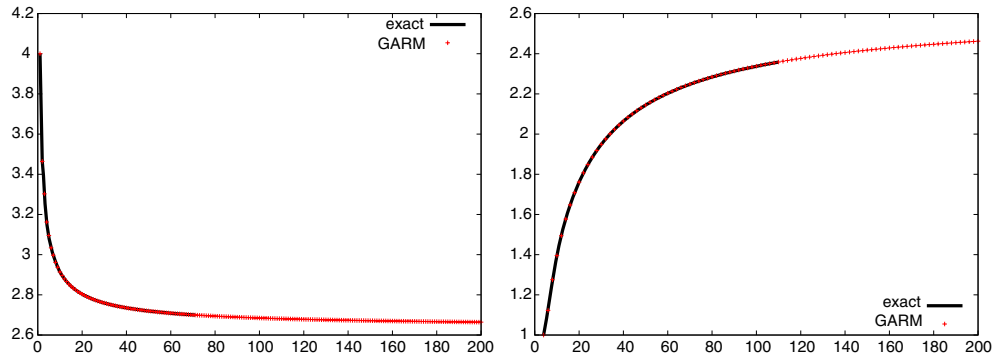
**The generalized atmospheric Rosenbluth method**

The generalized atmospheres,  $a_{\pm}$ , can be used to define a generalized Rosenbluth method for sampling SAWs. The algorithm starts with a single vertex,  $\varphi_0$ , and grows a sequence of SAWs,  $\varphi = \varphi_0, \dots, \varphi_n$ , by inserting a positive atmospheric edge at each iteration. The conformation  $\varphi_{k+1}$  is obtained from  $\varphi_k$  by inserting an edge chosen uniformly from the available positive atmospheric edges,  $a_+(\varphi_k)$ . We call this the generalized atmospheric Rosenbluth method (GARM). This method generalizes the percolation-based algorithms for trees in [17, 18].

A sequence of  $n + 1$  SAWs,  $\varphi = \varphi_0, \dots, \varphi_n$ , is obtained after  $n$  iterations with probability

$$\Pr(\varphi|\varphi_0) = \prod_{k=1}^n a_+(\varphi_{k-1})^{-1}. \tag{6}$$

Since a given conformation can be obtained in several different ways, this is *not* the probability of obtaining the last SAW in the sequence. As such we give a weight to the sequence of SAWs,



**Figure 5.** Left: a plot of  $c_n^{1/n}$  against length as estimated from GARM data up to length 200. Exact enumeration data up to length 71 taken from [19] are shown for comparison. Right: a plot of  $p_n^{1/n}$  against length as estimated from GARM data up to length 200 for even  $n$ . Exact enumeration data up to length 110 taken from [20] are shown for comparison.

not only to compensate for the non-uniform sampling probability, but also to take into account this degeneracy. The weight of a sequence of SAWs,  $\varphi = \varphi_0, \dots, \varphi_n$ , is

$$W(\varphi) = \prod_{k=1}^n \frac{a_+(\varphi_{k-1})}{a_-(\varphi_k)}, \tag{7}$$

if  $n \geq 1$  and  $W(\varphi) = 1$  if  $n = 0$ .

The mean weight of sequences of length  $n + 1$  is

$$\langle W \rangle_n = \sum_{\varphi} W(\varphi) \Pr(\varphi|\varphi_0) = c_n. \tag{8}$$

To see this, consider all the sequences that end in a particular SAW  $\tau$  of length  $n$ . It suffices to show that

$$1 = \sum_{\varphi \rightarrow \tau} W(\varphi) \Pr(\varphi|\varphi_0) = \sum_{\varphi \rightarrow \tau} \prod_{k=1}^n a_-(\varphi_k)^{-1}, \tag{9}$$

where the sums are over all sequences that end in  $\tau$ . Note that one must consider all the possible choices of atmospheric edges, so that there are  $n!$  sequences that end in the SAW made up of  $n$  east edges.

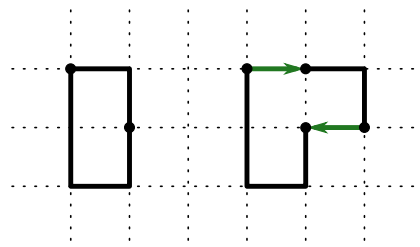
We reinterpret the product of negative atmospheres as the probability of returning to the single vertex under the following process. Starting at  $\varphi_n$ , we delete negative atmospheric edges from  $\varphi_k$  to obtain  $\varphi_{k-1}$  iteratively. The probability of realizing  $\varphi_0$  along the sequence  $\varphi$  is

$$\Pr(\varphi_0|\varphi) = \prod_{k=1}^n \Pr(\varphi_{k-1}|\varphi_k) = \prod_{k=1}^n a_-(\varphi_k)^{-1}. \tag{10}$$

Since all sequences that end in  $\tau$  must return to  $\varphi_0$  by this process, summing over  $\varphi$  gives equation (9) as required.

The above proof becomes trivial in the case of the endpoint atmosphere since  $a_- \equiv 1$  and each SAW is obtained in exactly one way. The proof breaks down in models in which a given conformation cannot be reached by inserting positive atmospheric edges.

In figure 5 (left), we show that data obtained by a pruned and enriched implementation of GARM for SAWs agree with exact enumeration data from [19]. We generated SAWs of a



**Figure 6.** A SAP and the insertion of a pair of anti-parallel edges. This SAP has the positive atmosphere of 21 and the negative atmosphere of 4.

maximum of 200 edges with approximately  $10^6$  trajectories consisting of a total of  $2.5 \times 10^8$  samples. This algorithm for the square lattice generalizes to SAWs on any graph with a finite maximal degree.

### Extensions to polygons, trees and animals

We now extend this algorithm to SAPs on the square lattice. In a previous paper, we defined the positive atmosphere to be the locations in which a single edge can be replaced by a  $\square$  conformation of three edges and the negative atmosphere was defined by the inverse of this process [21]. This definition is insufficient for GARM since there are many conformations that are not obtainable from the unit square—for example the  $2 \times 2$  square.

We generalize the notion of positive atmospheres of SAPs by considering all the pairs of vertices at which anti-parallel edges may be inserted to obtain a longer SAP. The negative atmosphere is defined by finding all pairs of edges that may be removed to obtain a SAP, see figure 6. All SAPs have non-zero positive atmosphere. Since the atmospheres now consist of pairs of edges we have

$$\frac{\langle a_+ \rangle_{2n}}{\langle a_- \rangle_{2n+2}} = \frac{p_{2n+2}}{p_{2n}}, \tag{11}$$

where  $p_{2n}$  is the number of SAPs of length  $2n$ .

In figure 5 (right), we show that data obtained by a PERM-like implementation of GARM for SAPs agree with exact enumeration data from [20]. We generated SAPs of a maximum of 200 edges with approximately  $4 \times 10^5$  trajectories consisting of a total of  $5 \times 10^7$  samples.

This algorithm does not simply generalize to three dimensions with this definition of atmospheres. If  $\varphi_0$  is chosen to be a unit square, then knotted conformations cannot be reached since inserting atmospheric edges does not allow strand passages. We are currently investigating how edge-deletion moves may be added to the GARM algorithm. This would enable the algorithm to reach all polygons of a given fixed knot type (just as the BFACF algorithm does [22]), and so allow us to do approximate enumeration of these objects.

GARM can be applied to the lattice bond tree model of branched polymers. The algorithm is then closely related to the algorithms in [17, 18, 23]. In this case, we define the positive atmosphere by looking at all the vertices at which an edge can be inserted to obtain a valid tree. When inserting an edge at a given vertex, one must be careful to consider all the possible ways of distributing the incident branches between both ends of the new edge. One may similarly define positive and negative atmospheres for animals. The positive atmosphere is defined by all the ways in which an edge may be inserted at vertices; unlike the tree case, some inserted edges will create cycles and so are double counted as they can be inserted from either vertex.

The negative atmosphere is defined by the inverse of this process and atmospheric edges that are not cut-edges will be double counted. This algorithm works for site trees; this may be easily implemented by defining positive and negative atmospheres in terms of leaves, but more general atmospheres are possible.

The implementation of the GARM algorithm requires rapid calculation of the positive and negative atmospheres. For SAWs the positive and negative atmospheres are  $O(n)$  while for SAPs they are  $O(n^2)$ . At present we are able to compute the atmospheres in  $O(n)$  time for SAWs and  $O(n^2)$  for SAPs. Since the atmospheres must be computed at each iteration, the time to produce a conformation of length  $n$  is  $O(n^2)$  and  $O(n^3)$  for SAWs and SAPs, respectively.

## Conclusions

The definitions of atmospheres above were limited to positive and negative since they either increase or decrease the number of edges. We can generalize this further by including the notion of neutral atmospheric moves,  $a_0$ , which change the conformation without changing its size—for example a pivot move. At each iteration the algorithm uniformly chooses to add an edge from the positive atmosphere or to apply a neutral atmospheric move. The probability of obtaining a sequence  $\varphi$  is

$$\Pr(\varphi|\varphi_0) = \prod_{k=1}^{|\varphi|-1} (a_+(\varphi_{k-1}) + a_0(\varphi_{k-1}))^{-1}, \quad (12)$$

and the corresponding weight is

$$W(\varphi) = \prod_{k=1}^{|\varphi|-1} \frac{a_+(\varphi_{k-1}) + a_0(\varphi_{k-1})}{a_-(\varphi_k) + a_0(\varphi_k)}, \quad (13)$$

where  $|\varphi|$  is the number of conformations in the sequence  $\varphi$ . The average weight of all sequences ending in a conformation of size  $n$  is  $c_n$ ; the proof is as above. This addition makes it possible to sample SAPs in three dimensions and higher since the pivot algorithm is ergodic [24].

The algorithm can also be adapted to include Boltzmann factors (as per [3, 25]) so as to compute free energies. Further extensions such as multicanonical or flat-histogram methods, such as those developed in [9, 10], are possible. We hope to be able to add edge-deletion moves to the algorithm so as to allow the approximate enumeration of polygons of fixed knot types. We are also currently investigating techniques to compute atmospheres more efficiently as this will improve the convergence of the GARM algorithm.

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## References

- [1] Hammersley J M and Morton K W 1954 *J. R. Stat. Soc. B* **16** 23–38
- [2] Rosenbluth M N and Rosenbluth A W 1955 *J. Chem. Phys.* **23** 356–62



- [3] Grassberger P 1997 *Phys. Rev. E* **56** 3682–93
- [4] de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
- [5] Rybenkov V, Cozzarelli N and Vologodskii A 1993 *Proc. Natl Acad. Sci. USA* **90** 5307
- [6] Gee M and Whittington S G 1997 *J. Phys. A: Math. Gen.* **30** L1–5
- [7] Marcone B, Orlandini E, Stella A and Zonta F 2007 *Phys. Rev. E* **75** 41105
- [8] Symanzik K 1969 *Local Quantum Theory* (New York: Academic)
- [9] Bachmann M and Janke W 2003 *Phys. Rev. Lett.* **91** 208105
- [10] Prellberg T and Krawczyk J 2004 *Phys. Rev. Lett.* **92** 120602
- [11] Causo M S, Coluzzi B and Grassberger P 2000 *Phys. Rev. E* **62** 3958–73
- [12] Krawczyk J, Owczarek A L and Prellberg T 2007 *J. Stat. Mech.: Theor. Exp.* P09016
- [13] Hsu H P, Paul W and Binder K 2007 *Macromol. Symp.* **252** 58–67
- [14] Rechnitzer A and van Rensburg E J Janse 2002 *J. Phys. A: Math. Gen.* **35** L605–12
- [15] van Rensburg E J Janse and Rechnitzer A 2003 *Phys. Rev. E* **67** 36116
- [16] van Rensburg E J Janse and Rechnitzer A 2004 *J. Phys. A: Math. Gen.* **37** 6875–98
- [17] Care C M and Ettelaie R 2000 *Phys. Rev. E* **62** 1397–1404
- [18] Hsu H P, Nadler W and Grassberger P 2005 *J. Phys. A: Math. Gen.* **38** 775–806
- [19] Jensen I 2004 *J. Phys. A: Math. Gen.* **37** 5503–24
- [20] Jensen I 2003 *J. Phys. A: Math. Gen.* **36** 5731–45
- [21] van Rensburg E J Janse and Rechnitzer A 2008 *J. Phys. A: Math. Theor.* **41** 105002
- [22] Janse van Rensburg E J and Whittington S G 1991 *J. Phys. A: Math. Gen.* **24** 5553–67
- [23] Meirovitch H 1987 *J. Phys. A: Math. Gen.* **20** 6059–73
- [24] Madras N, Orbitsky A and Shepp L A 1990 *J. Stat. Phys.* **58** 159–83
- [25] Seno F and Stella A L 1988 *J. Phys. France* **49** 739–48