# From Rosenbluth Sampling to PERM

rare event sampling with stochastic growth algorithms

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# Topic Outline

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# Sampling Algorithms

Markov Chain Monte Carlo (MCMC) Methods

- Transition from state $i$ to state $j$ with probability $P_{i,j}$
- Ergodicity
- Detailed Balance Condition for Equilibrium

$$\pi_i P_{i,j} = \pi_j P_{j,i}$$

- Normally fixed system size (e.g. constant number of spins)

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Stochastic Growth Methods

- No Markov Chain
- Grow independent configurations from scratch
- Incomplete enumeration

At each growth step, select one of all possible continuations

# Lattice paths

Relevant as model of polymer chains

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## Goal of these Lectures

Present growth algorithms with *uniform sampling* for lattice walks

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Distribution of endpoints

- walks end at position $k+(n-k)$ with probability

$$P_{n,k} = \frac{1}{2^n}\binom{n}{k}$$

($k$ steps to the right, $n-k$ steps to the left)

# Simple Sampling of Simple Random Walk

$s_{\cdot,\cdot} \leftarrow 0$
$Samples \leftarrow 0$
**while** $Samples < MaxSamples$ **do**
  $Samples \leftarrow Samples + 1$
  $n \leftarrow 0,\ k \leftarrow 0$
  $s_{0,0} \leftarrow s_{0,0} + 1$
  **while** $n < MaxLength$ **do**
    $n \leftarrow n + 1$
    Draw random number $r \in [0, 1]$
    **if** $r > 1/2$ **then**
      $k \leftarrow k + 1$
    **end if**
    $s_{n,k} \leftarrow s_{n,k} + 1$
  **end while**
**end while**

# Properties of Simple Sampling

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- Impossible to sample the tails of the distribution ($P_{n,0} = 2^{-n}$)

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How can we tweak the algorithm to reach the tails?

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# Biased Sampling

Introduce bias

- Jump to left with probability $p$
- Jump to right with probability $1 - p$

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$$P_{n,k} = \binom{n}{k} p^{n-k}(1-p)^k$$

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# Biased Sampling of Simple Random Walk

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$Samples \leftarrow 0$
**while** $Samples < MaxSamples$ **do**
  $Samples \leftarrow Samples + 1$
  $n \leftarrow 0$, $k \leftarrow 0$, $Weight \leftarrow 1$
  $s_{0,0} \leftarrow s_{0,0} + 1$, $w_{0,0} \leftarrow w_{0,0} + Weight$
  **while** $n < MaxLength$ **do**
    $n \leftarrow n + 1$
    Draw random number $r \in [0, 1]$
    **if** $r > p$ **then**
      $k \leftarrow k + 1$, $Weight \leftarrow Weight/2(1 - p)$
    **else**
      $Weight \leftarrow Weight/2p$
    **end if**
    $s_{n,k} \leftarrow s_{n,k} + 1$, $w_{n,k} \leftarrow w_{n,k} + Weight$
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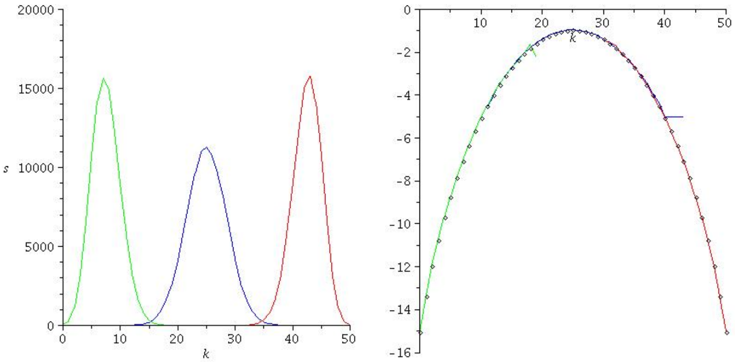


Biased sampling of simple random walk for $n = 50$ steps and bias $p = 0.85$ (green), $p = 0.5$ (blue), and $p = 0.15$ (red). For each simulation, 100000 samples were generated.

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- Need to choose different biases $p$ such that distributions overlap

Can we tweak the algorithm to avoid several simulations?

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# Uniform Sampling

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Allow for *local* biassing of random walk

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$$p_{n,k} = \frac{n+1-k}{n+2}$$

[EXERCISE]

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- replace global bias $p$ by local bias

$$p_{n,k} = \frac{n+1-k}{n+2}$$

[EXERCISE]

- Change weight of configuration by factor

$$1/2p_{n,k} \quad \text{or} \quad 1/2(1-p_{n,k})$$

# Uniform Sampling of Simple Random Walk

Initialize local biases

**for** $n = 0$ to $MaxLength$ **do**
  **for** $k = 0$ to $n$ **do**
    $p_{n,k} \leftarrow (n+1-k)/(n+2)$
  **end for**
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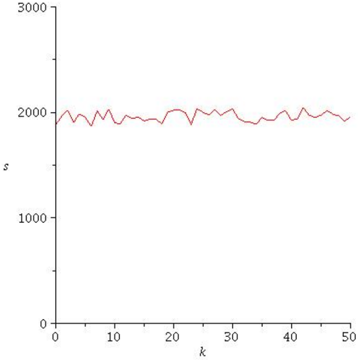
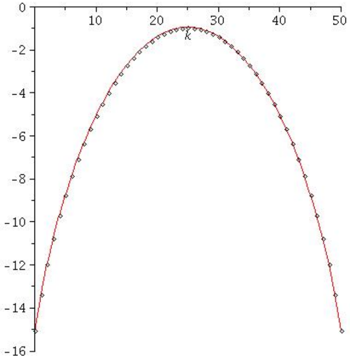
  **end for**
**end for**

and change the algorithm slightly

**if** $r > p_{n,k}$ **then**
  $k \leftarrow k+1,\ Weight \leftarrow Weight/2(1-p_{n,k})$
**else**
  $Weight \leftarrow Weight/2p_{n,k}$
**end if**




Uniform sampling of simple random walk for $n = 50$ steps, with 100000 samples generated.

# Properties of Uniform Sampling

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$$P_{n,k} = \frac{1}{n+1}$$

and has weight

$$W_{n,k} = \frac{n+1}{2^n} \binom{n}{k}$$

[Exercise]

- Distribution is perfectly uniform

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[Exercise]

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What if we don't know how to compute the biases $p_{n,k}$?

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Use this non-uniformity to iteratively tune weights

This works!

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## Pruning and Enrichment Strategy

- **Pruning** If the weight is too small, remove the configuration probabilistically
- **Enrichment** If the weight is too large, make several copies of the configuration

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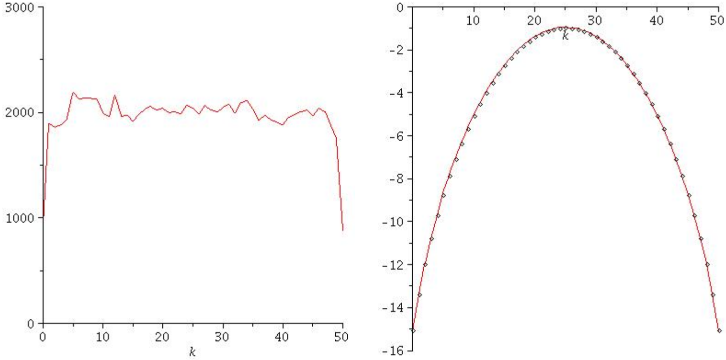
## Drawback of Pruning and Enrichment

- Need to deal with correlated data
- No a priori error analysis available
- A posteriori error analysis very difficult (only heuristics)

$Tours \leftarrow 0$, $n \leftarrow 0$, $k_0 \leftarrow 0$, $Weight_0 \leftarrow 1$
$s_{0,k_0} \leftarrow s_{0,k_0} + 1$, $w_{0,k_0} \leftarrow w_{0,k_0} + Weight_0$
**while** $Tours < MaxTours$ **do** {Main loop}
  **if** $n = MaxLength$ **then** {Maximal length reached: don't grow}
    $Copy_n \leftarrow 0$
  **else** {pruning/enrichment by comparing with target weight}
    $Ratio \leftarrow Weight_n / W_{n,k_n}$
    $p \leftarrow Ratio \mod 1$
    Draw random number $r \in [0,1]$
    **if** $r < p$ **then**
      $Copy_n \leftarrow \lfloor Ratio \rfloor + 1$
    **else**
      $Copy_n \leftarrow \lfloor Ratio \rfloor$
    **end if**
    $Weight_n \leftarrow w_{n,k_n}$
  **end if**
  **if** $Copy_n = 0$ **then** {Shrink to last enrichment point or to size zero}
    **while** $n > 0$ and $Copy_n = 0$ **do**
      $n \leftarrow n - 1$
    **end while**
  **end if**
  **if** $n = 0$ and $Copy_0 = 0$ **then** {start new tour}
    $Tours \leftarrow Tours + 1$, $n \leftarrow 0$, $k_0 \leftarrow 0$, $Weight_0 \leftarrow 1$
    $s_{n,k_n} \leftarrow s_{n,k_n} + 1$, $w_{n,k_n} \leftarrow w_{n,k_n} + Weight_n$
  **else** {Grow by one step}
    $Copy_n \leftarrow Copy_n - 1$
    Draw random number $r \in [0,1]$
    **if** $r > 1/2$ **then**
      $k_{n+1} \leftarrow k_n + 1$
    **else**
      $k_{n+1} \leftarrow k_n$
    **end if**
    $Weight_{n+1} \leftarrow Weight_n$, $n \leftarrow n + 1$
    $s_{n,k_n} \leftarrow s_{n,k_n} + 1$, $w_{n,k_n} \leftarrow w_{n,k_n} + Weight_n$
  **end if**
**end while**

# Pruned and Enriched Sampling of Simple Random Walk

**repeat**
    **if** maximal lenght reached **then**
        set number of enrichment copies to zero
    **else**
        prune/enrich step: compute number of enrichment copies
    **end if**
    **if** number of enrichment copies is zero **then**
        prune: shrink to previous enrichment
    **end if**
    **if** configuration shrunk to zero **then**
        start new tour
        store data for new configuration
    **else**
        decrease number of enrichment copies
        grow new step
        store data for new configuration
    **end if**
**until** enough data is generated




Pruned and enriched sampling of simple random walk for $n = 50$ steps, with 100000 tours generated.

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- insert

  $W_{n,k_n} \leftarrow (n+1)w_{n,k_n}/\sum_l w_{n,l}$

  just before

  $Ratio \leftarrow Weight_n/W_{n,k_n}$

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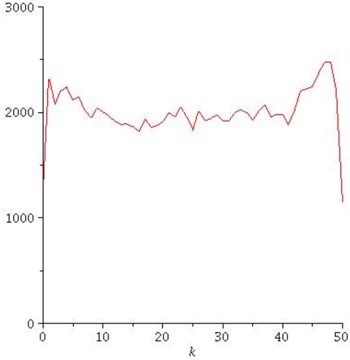
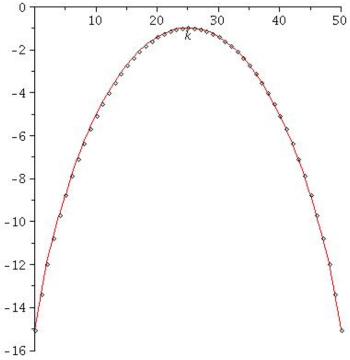
That's all!




Blind pruned and enriched sampling of simple random walk for $n = 50$ steps, with 100000 tours generated.

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Anyone interested?

# Summary of First Lecture

Sampling of Random Walks

- Simple Sampling
- Biased Sampling
- Uniform Sampling
- Pruned and Enriched Sampling
- Blind Pruned and Enriched Sampling

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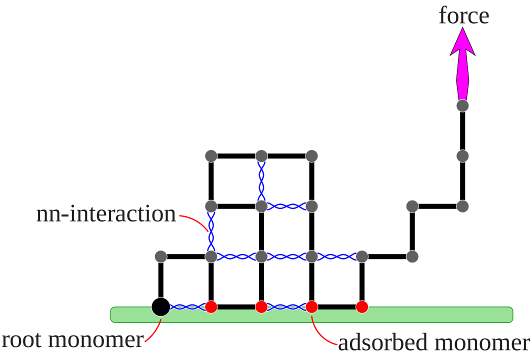
Slightly unrealistic situation because

- Random walks never trap - no attrition!

# Outline

# "Realistic" Lattice Models of Polymers




A self-avoiding walk lattice model of a polymer tethered to a sticky surface under the influence of a pulling force.

# The Effect of Self-Avoidance

Physically,

- Excluded volume changes the universality class

[1] N Clisby, PRL **104** 055702 (2010), using the Pivot Algorithm

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- Different critical exponents, e.g. length scale exponent changes

$$R \sim n^{\nu}$$

where $\nu = 0.5$ for RW and $\nu = 0.587597(7)\ldots$[1] for SAW in d=3

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and mathematically,

- Self-avoidance turns a simple Markovian random walk without memory into a complicated non-Markovian random walk with infinite memory
- When growing a self-avoiding walk, one needs to test for self-intersection with all previous steps

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# Simple Sampling of Self-Avoiding Walk

From now on, consider Self-Avoiding Walks (SAW) on $\mathbb{Z}^2$

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From now on, consider Self-Avoiding Walks (SAW) on $\mathbb{Z}^2$

- Simple sampling of SAW works just like simple sampling of random walks
- But now walks get removed if they self-intersect

# Simple Sampling of Self-Avoiding Walk

$s_{.} \leftarrow 0$
$Samples \leftarrow 0$
**while** $Samples < MaxSamples$ **do**
  $Samples \leftarrow Samples + 1$
  $n \leftarrow 0$, Start at origin
  $s_0 \leftarrow s_0 + 1$
  **while** $n < MaxLength$ **do**
    Draw one of the neigboring sites uniformly at random
    **if** Occupied **then**
      Reject entire walk and exit loop
    **else**
      Step to new site
      $n \leftarrow n + 1$
      $s_n \leftarrow s_n + 1$
    **end if**
  **end while**
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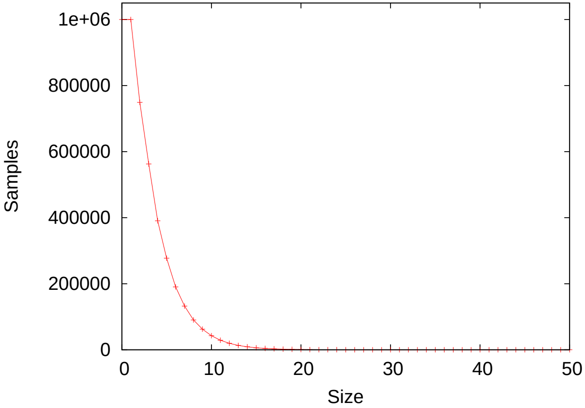
This is called exponential attrition




Attrition of started walks generated with Simple Sampling. From $10^6$ started walks none grew more than 35 steps.

# Outline

# Rosenbluth Sampling

A slightly improved sampling algorithm was proposed in 1955 by Rosenbluth and Rosenbluth[2].

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Configurations are generated with varying probabilities, depending on the number of ways they can be continued

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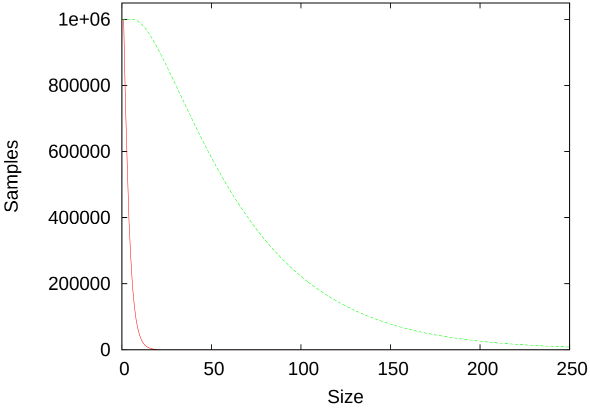
An $n$-step walk grown by Rosenbluth sampling therefore has weight

$$W_n = \prod_{i=0}^{n-1} a_i$$

and is generated with probability $P_n = 1/W_n$, so that $P_n W_n = 1$ as required.

# Rosenbluth Sampling of Self-Avoiding Walk

$Samples \leftarrow 0$
**while** $Samples < MaxSamples$ **do**
  $Samples \leftarrow Samples + 1$
  $n \leftarrow 0$, $Weight \leftarrow 1$, Start at origin
  $s_0 \leftarrow s_0 + 1$, $w_0 \leftarrow w_0 + Weight$
  **while** $n < MaxLength$ **do**
    Create list of neighboring unoccupied sites
    Determine the atmosphere $a$
    **if** $a = 0$ (walk cannot continue) **then**
      Reject entire walk and exit loop
    **else**
      Step to one of the unoccupied sites
      $n \leftarrow n + 1$, $Weight \leftarrow Weight \times a$
      $s_n \leftarrow s_n + 1$, $w_n \leftarrow w_n + Weight$
    **end if**
  **end while**
**end while**




Attrition of started walks generated with Rosenbluth Sampling compared with Simple Sampling.

# Outline

# Pruned and Enriched Rosenbluth Sampling

- No significant improvements for four decades

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- For details, and several enhancements of PERM see review paper[4]

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# Pruned and Enriched Rosenbluth Sampling

**repeat**
  **if** zero atmosphere or maximal lenght reached **then**
    set number of enrichment copies to zero
  **else**
    prune/enrich step: compute number of enrichment copies
  **end if**
  **if** number of enrichment copies is zero **then**
    prune: shrink to previous enrichment
  **end if**
  **if** configuration shrunk to zero **then**
    start new tour and store data for new configuration
  **else**
    decrease number of enrichment copies
    **if** positive atmosphere **then**
      grow new step and store data for new configuration
    **end if**
  **end if**

$Tours \longleftarrow 0$, $n \longleftarrow 0$, $Weight_0 \longleftarrow 1$
Start new walk with step size zero
$a \longleftarrow 0$, $Copy_0 \longleftarrow 1$
$s_0 \longleftarrow s_0 + 1$, $w_0 \longleftarrow w_0 + Weight$
**while** $Tours < MaxTours$ **do** {Main loop}
  **if** $n = MaxLength$ or $a = 0$ **then** {Maximal length reached or atmosphere zero: don't grow}
    $Copy_n \longleftarrow 0$
  **else** {pruning/enrichment by comparing with target weight}
    $Ratio \longleftarrow Weight_n / w_n$
    $p \longleftarrow Ratio \mod 1$
    Draw random number $r \in [0, 1]$
    **if** $r < p$ **then**
      $Copy_n \longleftarrow \lfloor Ratio \rfloor + 1$
    **else**
      $Copy_n \longleftarrow \lfloor Ratio \rfloor$
    **end if**
    $Weight_n \longleftarrow w_n$
  **end if**
  **if** $Copy_n = 0$ **then** {Shrink to last enrichment point or to size zero}
    **while** $n > 0$ and $Copy_n = 0$ **do**
      Delete last site of walk
      $n \longleftarrow n - 1$
    **end while**
  **end if**
  **if** $n = 0$ and $Copy_0 = 0$ **then** {start new tour}
    $Tours \longleftarrow Tours + 1$,
    Start new walk with step size zero
    $a \longleftarrow 0$, $Copy_0 \longleftarrow 1$
    $s_0 \longleftarrow s_0 + 1$, $w_0 \longleftarrow w_0 + Weight$
  **else**
    Create list of neighboring unoccupied sites, determine the atmosphere $a$
    **if** $a > 0$ **then**
      $Copy_n \longleftarrow Copy_n - 1$
      Draw one of the neigboring unoccupied sites uniformly at random
      Step to new site
      $n \longleftarrow n + 1$, $Weight_n \longleftarrow Weight_n \times a$
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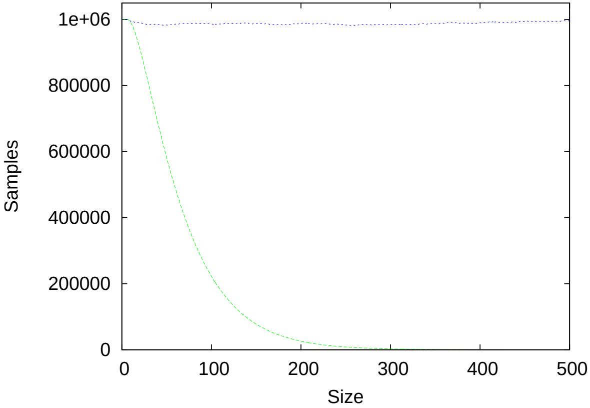


Attrition of started walks with PERM compared with Rosenbluth Sampling.

# Outline

# Interacting Self-Avoiding Walks

Consider sampling with respect to an extra parameter, for example the number of nearest-neighbour contacts

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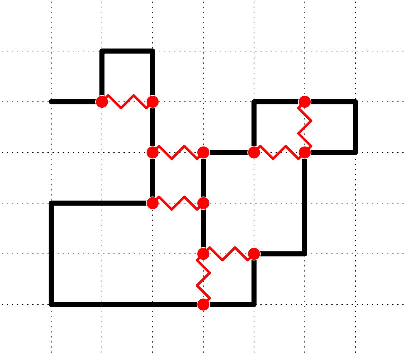

An interacting self-avoiding walk on the square lattice with $n = 26$ steps and $m = 7$ contacts.

# Uniform Sampling

Renewed interest in Uniform Sampling Algorithms

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Incorporating uniform sampling into PERM is straightforward, once one observes that PERM already samples uniformly *in system size*

# Flat Histogram Rosenbluth Sampling

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  $s_{n,m} \leftarrow s_{n,m} + 1,\ w_{n,m} \leftarrow w_{n,m} + Weight_n$

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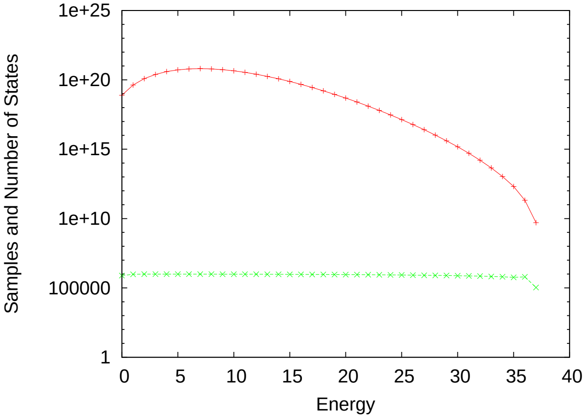
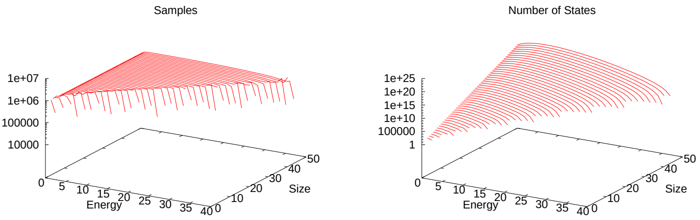
And that is all!




Generated samples and estimated number of states for ISAW with 50 steps estimated from $10^6$ flatPERM tours.




Generated samples and estimated number of states for ISAW with up to 50 steps generated with flatPERM.

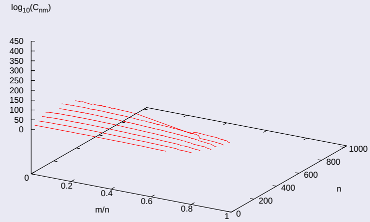
# Outline

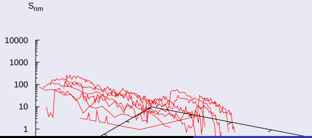
# 2d ISAW simulation up to $N = 1024$

To stabilise algorithm (avoid initial overflow/underflow):
Delay growth of large configurations
Here: after $t$ tours growth up to length $10t$

# 2d ISAW simulation up to $N = 1024$

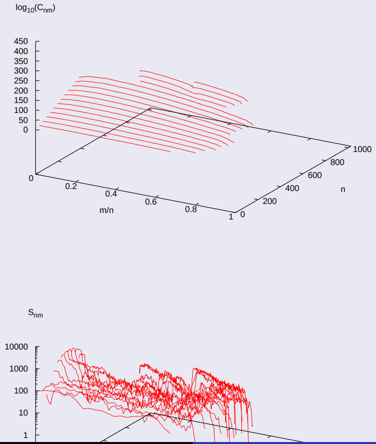
## Total sample size: $1,000,000$



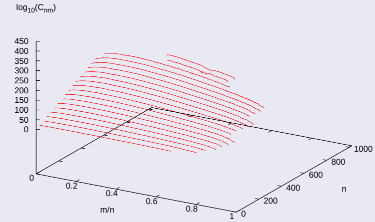
# 2d ISAW simulation up to $N = 1024$

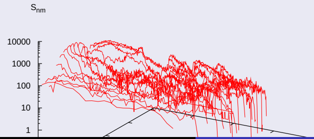
## Total sample size: $10,000,000$



# 2d ISAW simulation up to $N = 1024$

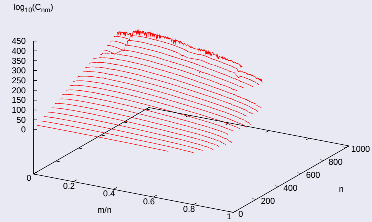
## Total sample size: $20,000,000$

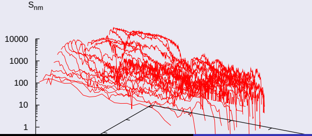


# 2d ISAW simulation up to $N = 1024$

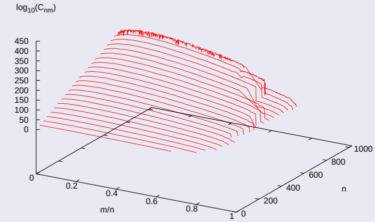
## Total sample size: $30,000,000$

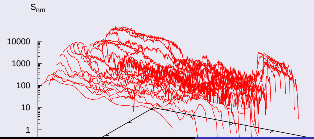


# 2d ISAW simulation up to $N = 1024$

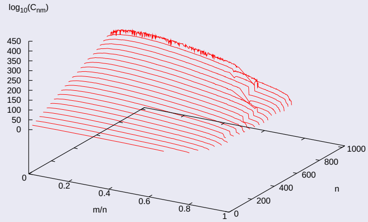
## Total sample size: $40,000,000$

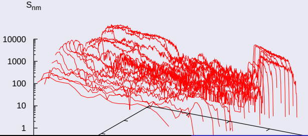


# 2d ISAW simulation up to $N = 1024$

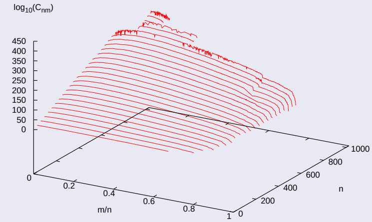
## Total sample size: $50,000,000$

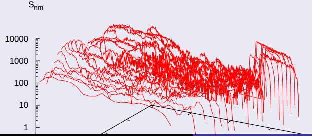


# 2d ISAW simulation up to $N = 1024$

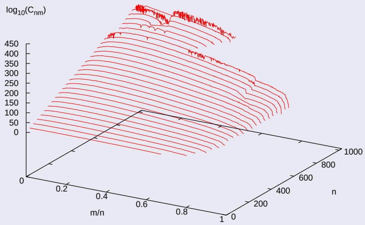
## Total sample size: $60,000,000$

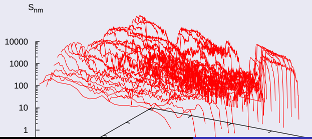


# 2d ISAW simulation up to $N = 1024$

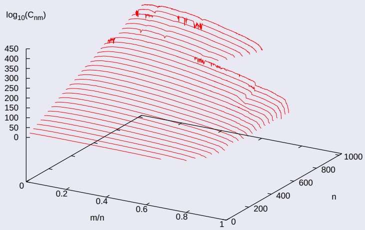
## Total sample size: $70,000,000$

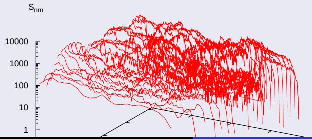


# 2d ISAW simulation up to $N = 1024$

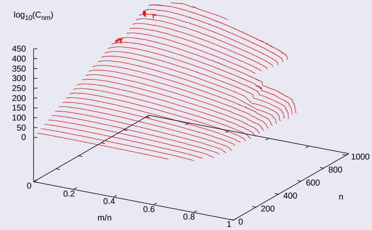
## Total sample size: $80,000,000$

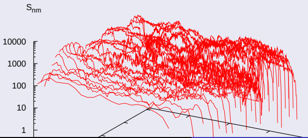


# 2d ISAW simulation up to $N = 1024$

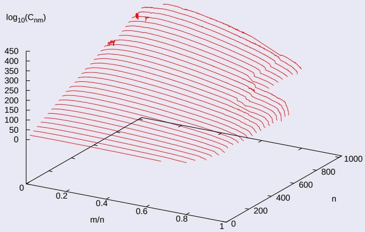
## Total sample size: $90,000,000$

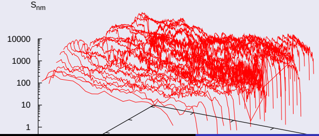


# 2d ISAW simulation up to $N = 1024$

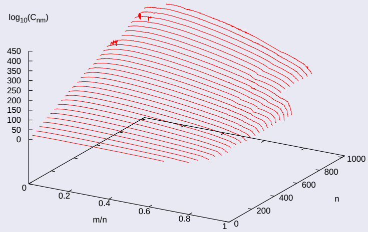
## Total sample size: $100,000,000$

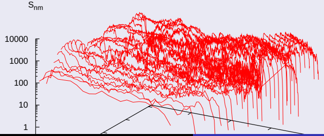


# 2d ISAW simulation up to $N = 1024$

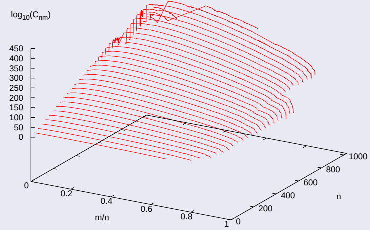
## Total sample size: $110,000,000$

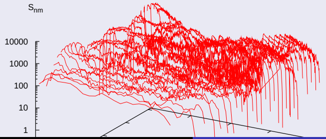


# 2d ISAW simulation up to $N = 1024$

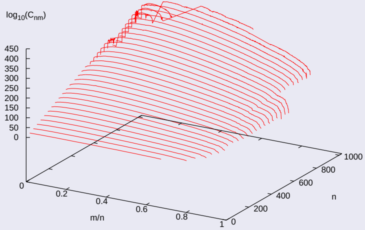
## Total sample size: $120,000,000$

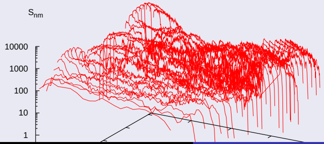


# 2d ISAW simulation up to $N = 1024$

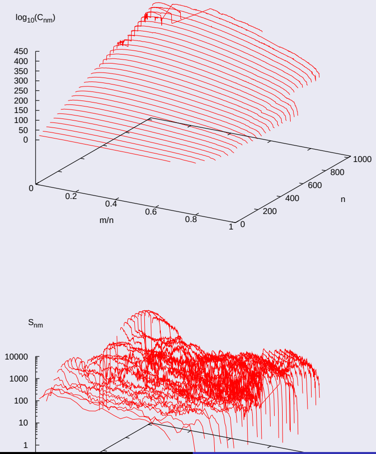
## Total sample size: $130,000,000$



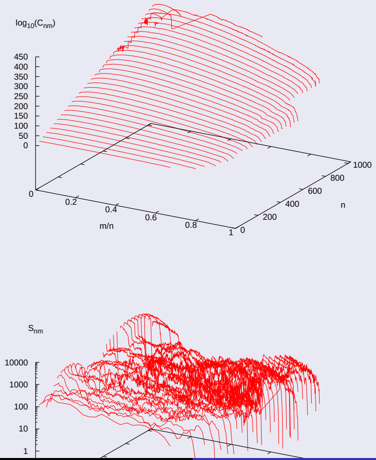
# 2d ISAW simulation up to $N = 1024$

## Total sample size: $140,000,000$



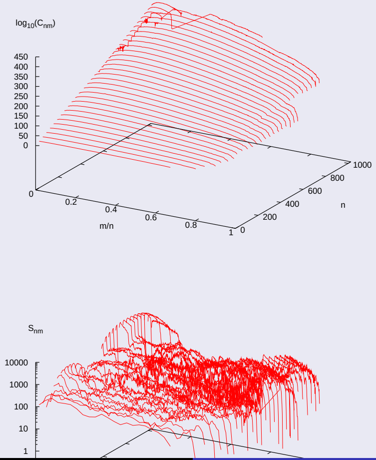
# 2d ISAW simulation up to $N = 1024$

## Total sample size: $150,000,000$



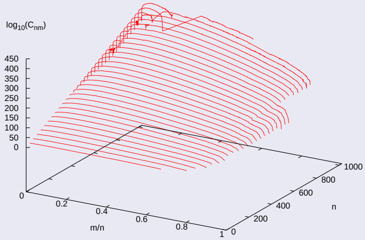
# 2d ISAW simulation up to $N = 1024$

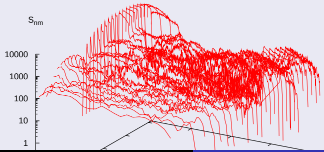
## Total sample size: $160,000,000$



# 2d ISAW simulation up to $N = 1024$

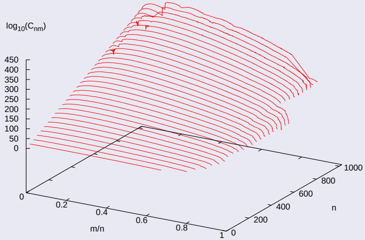
## Total sample size: $170,000,000$

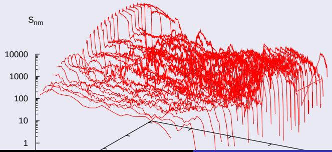


# 2d ISAW simulation up to $N = 1024$

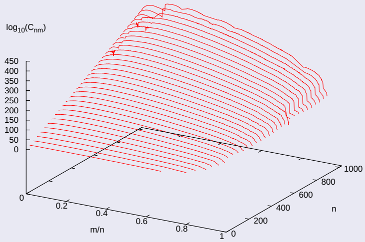
## Total sample size: $180,000,000$

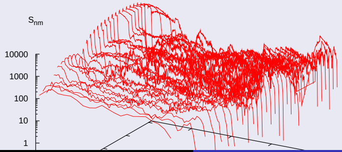


# 2d ISAW simulation up to $N = 1024$

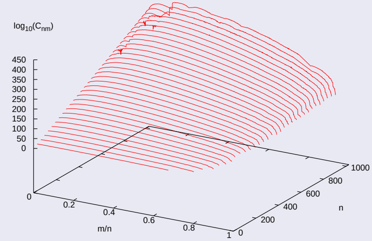
## Total sample size: $190,000,000$

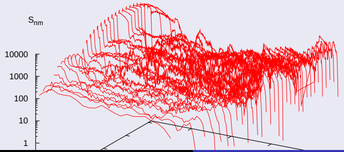


# 2d ISAW simulation up to $N = 1024$

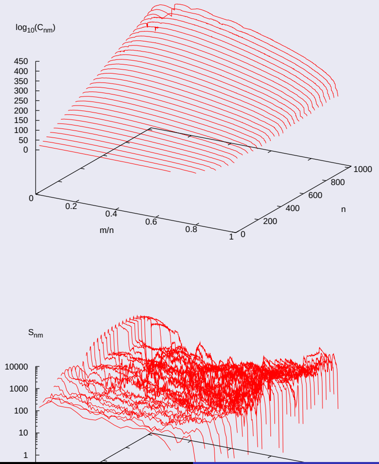
## Total sample size: $200,000,000$



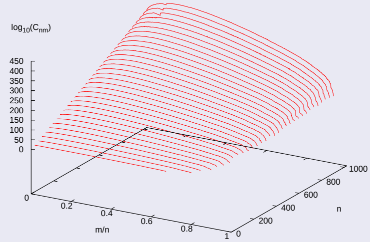
# 2d ISAW simulation up to $N = 1024$

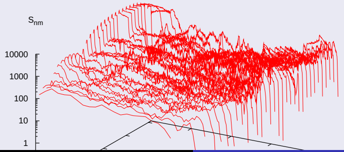
## Total sample size: $210,000,000$



# 2d ISAW simulation up to $N = 1024$

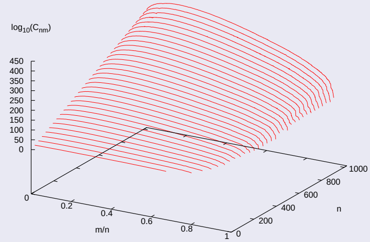
## Total sample size: $220,000,000$

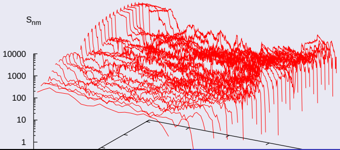


# 2d ISAW simulation up to $N = 1024$

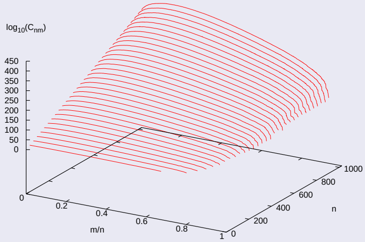
## Total sample size: $230,000,000$

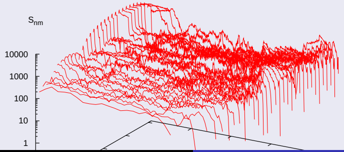


# 2d ISAW simulation up to $N = 1024$

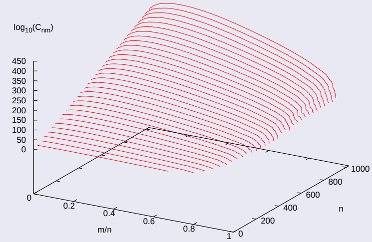
## Total sample size: $240,000,000$

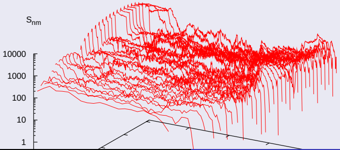


# 2d ISAW simulation up to $N = 1024$

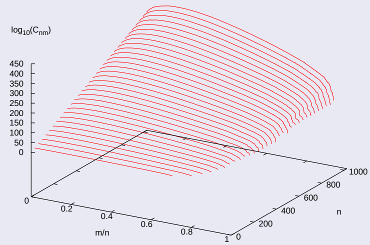
## Total sample size: $250,000,000$

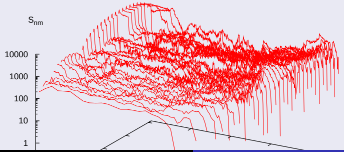


# 2d ISAW simulation up to $N = 1024$

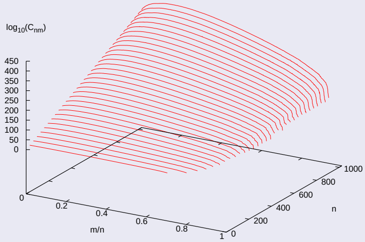
## Total sample size: $260,000,000$

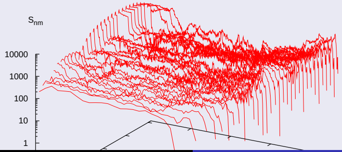


# 2d ISAW simulation up to $N = 1024$

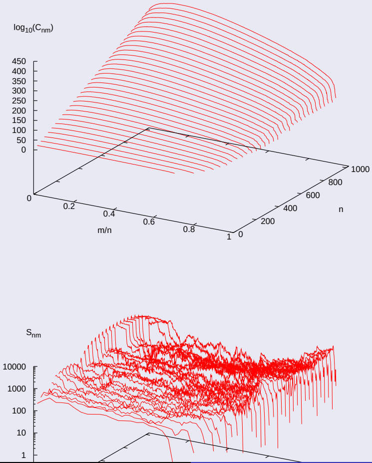
## Total sample size: $270,000,000$



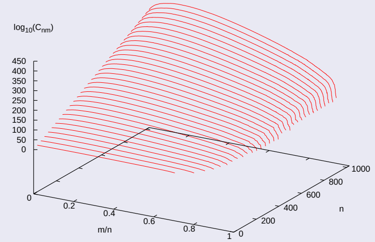
# 2d ISAW simulation up to $N = 1024$

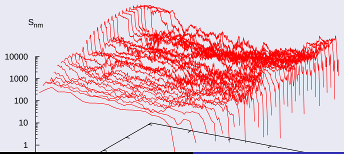
## Total sample size: $280,000,000$



# 2d ISAW simulation up to $N = 1024$

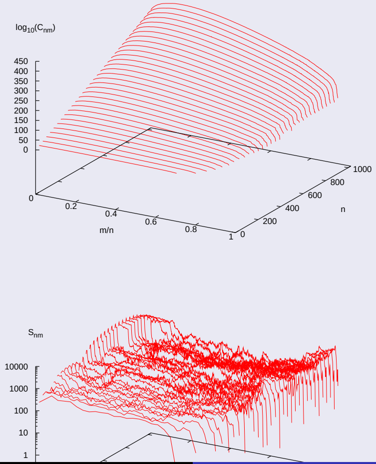
## Total sample size: $290,000,000$



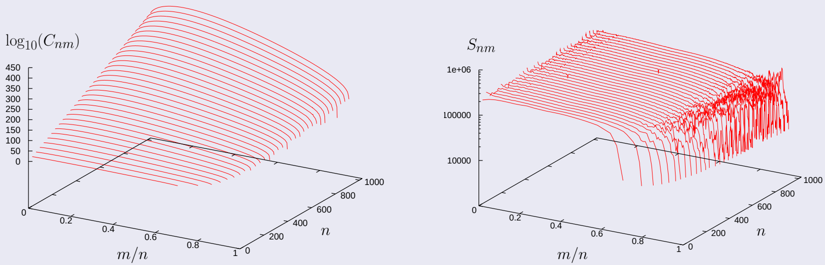
# 2d ISAW simulation up to $N = 1024$

## Total sample size: $300,000,000$



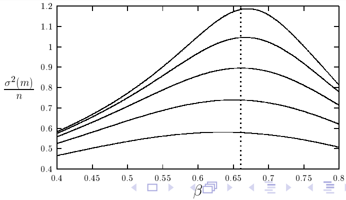
# ISAW simulations

T Prellberg and J Krawczyk, PRL 92 (2004) 120602




- 2d ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude

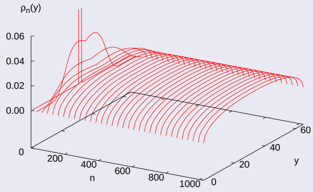
(only 2d shown, 3d similar)

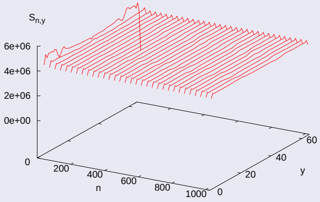


# Simulation results: SAW in a strip

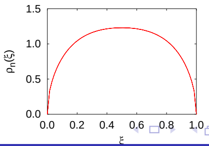
T Prellberg et al, in: Computer Simulation Studies in Condensed Matter Physics XVII, Springer Verlag, 2006

- 2d SAW in a strip: strip width 64, up to $n = 1024$



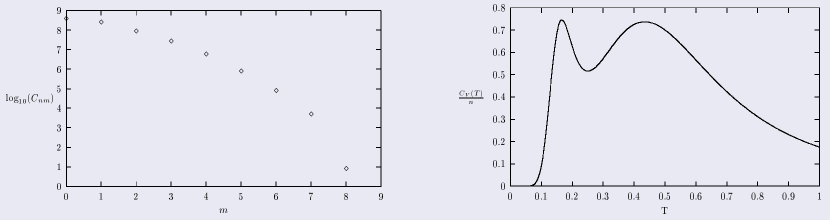

- Scaled endpoint density



# HP model simulations

T Prellberg et al, in: Computer Simulation Studies in Condensed Matter Physics XVII, Springer Verlag, 2006

- Engineered sequence HPHPHHPHPHHPPH in $d = 3$:




- Investigated other sequences up to $N \approx 100$ in $d = 2$ and $d = 3$
- Collapsed regime accessible
- Reproduced known ground state energies
- Obtained density of states $C_{n,m}$ over large range ($\approx 10^{30}$)

# Outline

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PERM (and its flat histogram version) can be applied objects that are grown in a unique way

- prime example: linear polymers

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What about objects that can be grown in different, not necessarily unique, ways?

- examples: ring polymers, branched polymers (lattice trees)

# Outline

# Positive and Negative Atmospheres

A. Rechnitzer and E. J. Janse van Rensburg, J. Phys. A **41** 442002 (2008)

## Key idea

Introduce an additional negative atmosphere $a^-$ indicating in how many ways a configuration can be reduced in size

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**Key idea**

Introduce an additional negative atmosphere $a^{-}$ indicating in how many ways a configuration can be reduced in size

- For linear polymers the negative atmosphere is always unity, as there is only one way to remove a step
- For lattice trees the negative atmosphere is equal to the number of its leaves

# Generalized Atmospheric Rosenbluth Sampling

A new algorithm: Generalized Atmospheric Rosenbluth Method (GARM)

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where $a_i$ are the (positive) atmospheres of the configuration after $i$ growth steps, and $a^-_i$ are the negative atmospheres of the configuration after $i$ growth steps.

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  where $a_i$ are the (positive) atmospheres of the configuration after $i$ growth steps, and $a^-_i$ are the negative atmospheres of the configuration after $i$ growth steps.
- The probability of growing this configuration is $P_n = 1/W_n$, so again $P_n W_n = 1$ holds as required.

# Generalized Atmospheric Rosenbluth Sampling

**while** $Samples < MaxSamples$ **do**
  $Samples \leftarrow Samples + 1$
  $n \leftarrow 0$, $Weight \leftarrow 1$, Start with seed configuration
  $s_0 \leftarrow s_0 + 1$, $w_0 \leftarrow w_0 + Weight$
  **while** $n < MaxSize$ **do**
    Create list of growth possibilities, determine the atmosphere $a$
    **if** $a = 0$ (no growth possible) **then**
      Reject entire configuration and exit loop
    **else**
      Draw one of the growth possibilities uniformly at random
      Grow configuration
      $n \leftarrow n + 1$, $Weight \leftarrow Weight \times a$
      Compute negative atmosphere $a^-$
      $Weight \leftarrow Weight / a^-$
      $s_n \leftarrow s_n + 1$, $w_n \leftarrow w_n + Weight$
    **end if**
  **end while**
**end while**

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- grow and shrink independently (Generalized Atmospheric Sampling, GAS)

For further extensions to Rosenbluth sampling, and indeed many more algorithms for simulating self-avoiding walks, as well as applications, see the review "Monte Carlo methods for the self-avoiding walk," E. J. Janse van Rensburg, J. Phys. A **42** 323001 (2009)