Rare event sampling with stochastic growth algorithms

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CAIMS 2012
June 24-28, 2012

Topic Outline

Outline

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Simple Random Walk in One Dimension

Model of directed polymer in $1 + 1$ dimensions

- Start at origin and step to left or right with equal probability
- 2^n possible random walks with n steps
- each walk generated with equal weight

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)

Properties of Simple Sampling

- Samples grown independently from scratch
- Each sample of an n-step walk is grown with equal probability
- 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?

Outline

Biased Sampling

Introduce bias

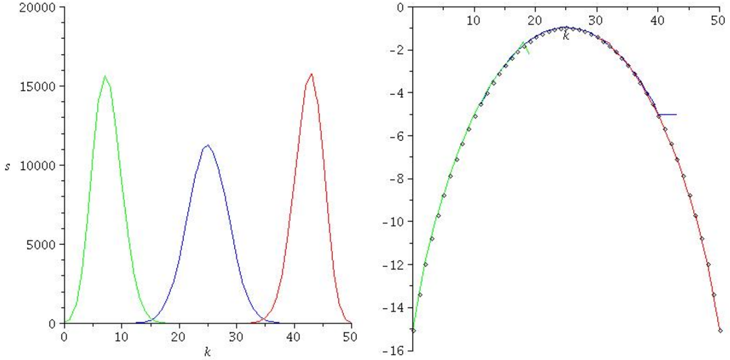
- Jump to left with probability p
- Jump to right with probability $1 - p$

Distribution of endpoints

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

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

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



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.

Properties of Biased Sampling

- Samples grown independently from scratch
- Each sample of an n-step walk ending at position k is grown with equal probability
- Distributions concentrated around $k = pn$ with width $O(\sqrt{n})$

- To cover the whole distribution, need $O(\sqrt{n})$ individual simulations
- Need to choose different biases p such that distributions overlap

Can we tweak the algorithm to avoid several simulations?

Outline

Uniform Sampling

Main Idea

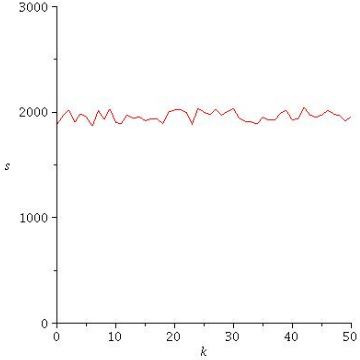
Allow for *local* biassing of random walk

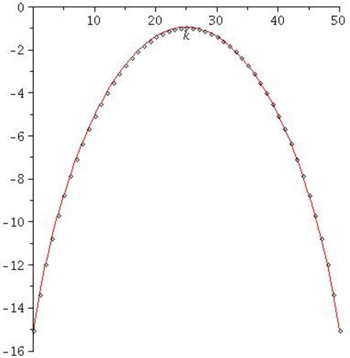
- replace global bias p by local bias

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

- 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 for $n = 50$ steps, with 100000 samples generated.

Properties of Uniform Sampling

- Samples grown independently from scratch
- Each sample of an n-step walk ending at position k is grown with equal probability
$$P_{n,k} = \frac{1}{n+1}$$
and has weight
$$W_{n,k} = \frac{n+1}{2^n}\binom{n}{k}$$
- Distribution is perfectly uniform
- One simulation suffices

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

Outline

From Biases to Weights: A Change of View

- Correct choice of local biases $p_{n,k}$ achieves uniform sampling
- If local biases are incorrect, sampling will be non-uniform

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Better Idea

Use this non-uniformity to iteratively tune weights

This works!

Pruned and Enriched Sampling

- For uniform sampling we need to achieve

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

- Simple sampling generates samples with weight $W_{n,k} = 2^{-n}$

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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

Pruning and Enrichment (ctd)

Suppose a walk has been generated with weight w, but ought to have target weight $W_{n,k}$.

- Compute ratio $R = w/W_{n,k}$
- If $R = 1$, do nothing
- If $R < 1$, stop growing with probability $1 - R$
- If $R > 1$, make $\lfloor R \rfloor + 1$ copies with probability $p = R - \lfloor R \rfloor$ and $\lfloor R \rfloor$ copies with probability $1 - p$
- Continue growing with weight w set to target weight W

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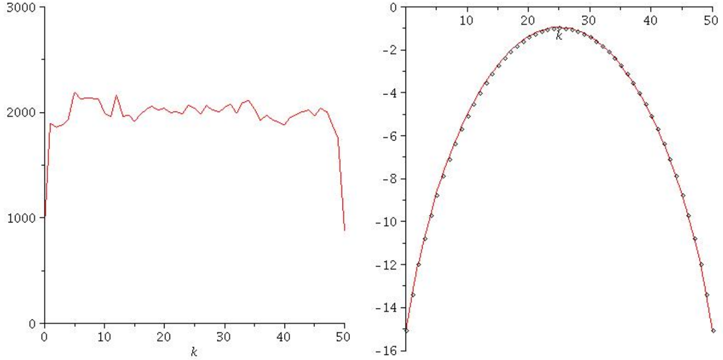
Drawback of Pruning and Enrichment

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



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

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- For a truly blind algorithm, need to also estimate target weights

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Key idea

Compute target weights on the fly

Replace exact weight $W_{n,k}$ by estimate $\langle W_{n,k} \rangle$ generated from data

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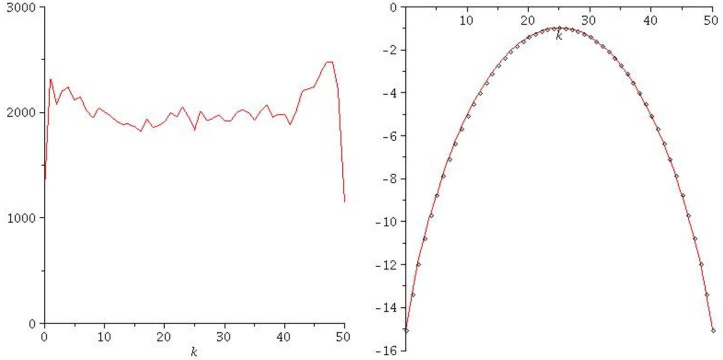
That's all!



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

Algorithm Analysis Needed!

- Any fixed choice of the target weight $W_{n,k}$ gives an algorithm that samples correctly (just maybe not that well)
- Replacing the optimal choice of $W_{n,k}$ by an estimate should converge to the optimal choice, hence lead to uniform sampling
- This is confirmed by simulations

The algorithm ought to be simple enough for a rigorous analysis

Summary so far

Sampling of Random Walks

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

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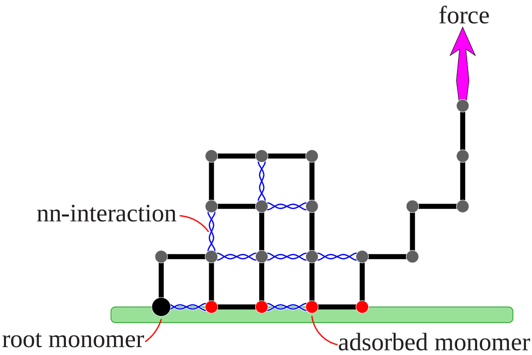
Slightly unrealistic situation because

- 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
- 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

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

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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

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

Outline

Simple Sampling of Self-Avoiding Walk

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

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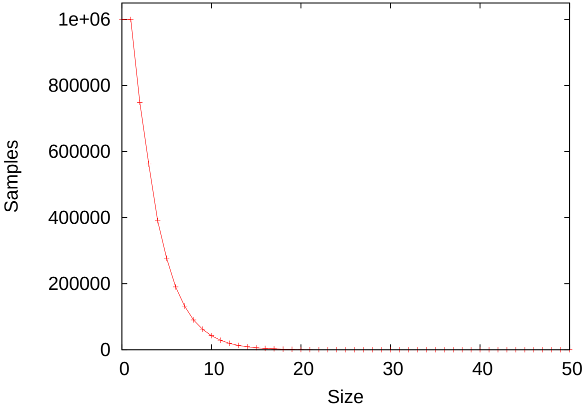
However

Generating SAW with simple sampling is very inefficient

- There are 4^n n-step random walks, but only about 2.638^n n-step SAW

This leads to 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].

- Avoid self-intersections by only sampling from the steps that don't self-intersect
- The growth only terminates if the walk is trapped and cannot continue growing

Still exponential attrition (albeit less)

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

[2] M. N. Rosenbluth and A. W. Rosenbluth, J. Chem. Phys. **23** 356 (1955)

The “Atmosphere” of a configuration

We call *atmosphere* a of a configuration the number of ways in which a configuration can continue to grow.

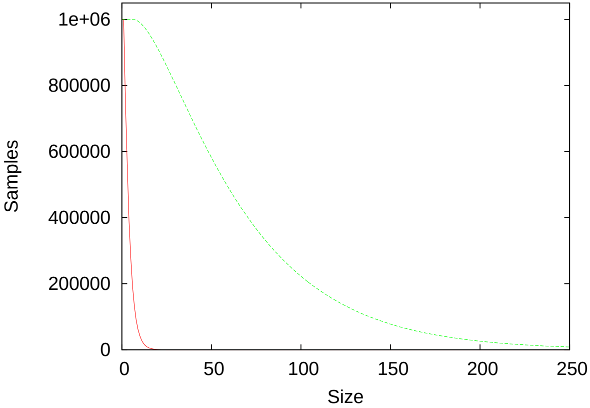
- For simple random walks, the atmosphere is constant
- For 2-dim SAW, the atmosphere varies between $a = 4$ (seed) and $a = 0$ (trapped)

If a configuration has atmosphere a then there are a different possibilities of growing the configuration, and each of these can get selected with probability $p = 1/a$, therefore the weight gets multiplied by a.

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.



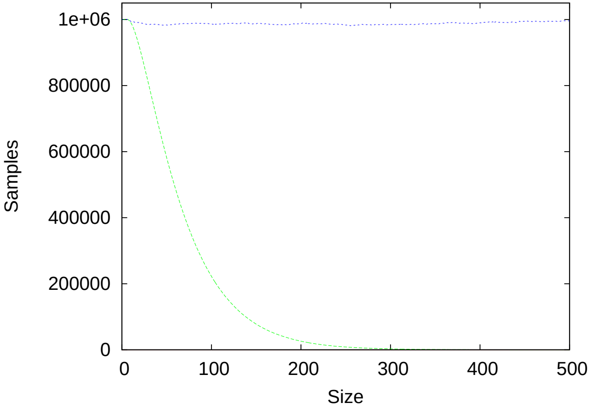
Attrition of started walks generated with Rosenbluth Sampling compared with Simple Sampling.

Outline

Pruned and Enriched Rosenbluth Sampling

- No significant improvements for four decades
- In 1997 Grassberger augmented Rosenbluth sampling with pruning and enrichment strategies[3]
- Grassberger's Pruned and Enriched Rosenbluth Method (PERM) uses somewhat different strategies from those presented here
- For details, and several enhancements of PERM see review papers[4,5]

[3] P. Grassberger, Phys. Rev E **56** 3682 (1997)
[4] E. J. Janse van Rensburg, J. Phys. A **42** 323001 (2009)
[5] H. P. Hsu and P. Grassberger, J. Stat. Phys. **144** 597 (2011)



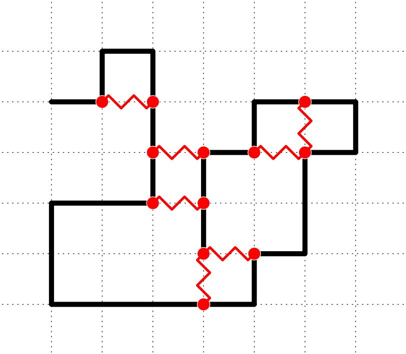
Attrition of started walks with PERM compared with Rosenbluth Sampling.

Outline

1. Sampling of Simple Random Walks
   - Simple Sampling
   - Biased Sampling
   - Uniform Sampling
   - Pruned and Enriched Sampling
   - Blind Pruned and Enriched Sampling
2. Sampling of Self-Avoiding Walks
   - Simple Sampling
   - Rosenbluth Sampling
   - Pruned and Enriched Rosenbluth Sampling
   - Flat Histogram Rosenbluth Sampling
   - Applications
3. Extensions
   - Generalized Atmospheric Rosenbluth Sampling

Interacting Self-Avoiding Walks

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



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

F. Wang and D. P. Landau, PRL **86** 2050 (2001)

- Multicanonical PERM

  M. Bachmann and W. Janke, PRL **91** 208105 (2003)
- Flat Histogram PERM

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

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

Flat Histogram Rosenbluth Sampling

Extension of PERM to a microcanonical version

- Distinguish configurations of size n by some additional parameter m (e.g. energy)
- Bin data with respect to n and m

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

- Enrichment ratio for pruning/enrichment becomes

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

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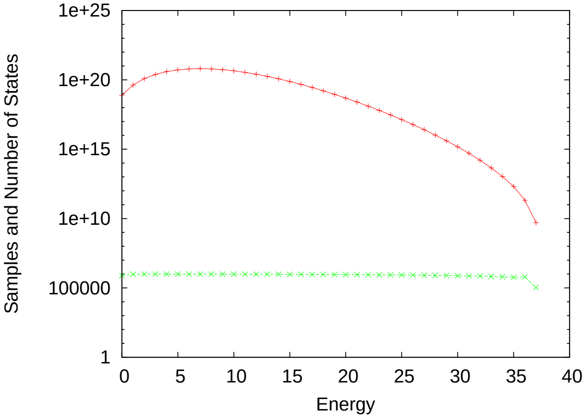
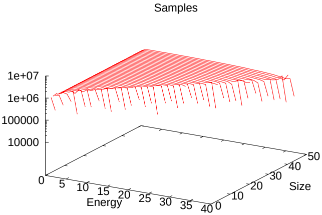
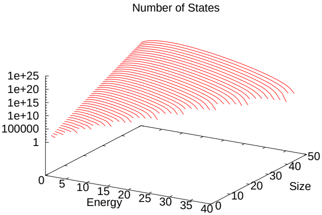
And that is all!



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



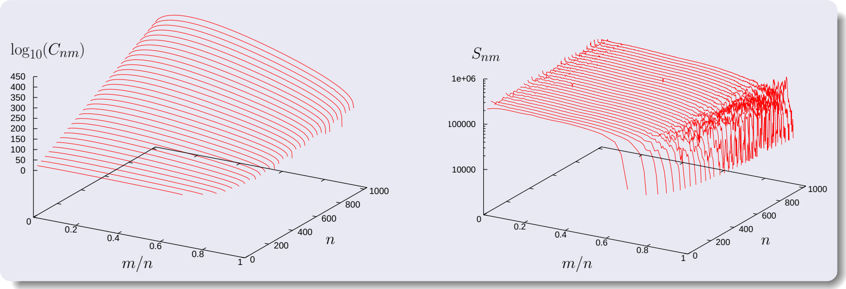


Generated samples and estimated number of states for ISAW with up to 50 steps generated with flatPERM.

Outline

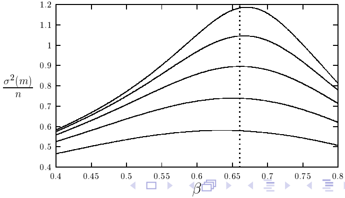
ISAW simulations

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



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

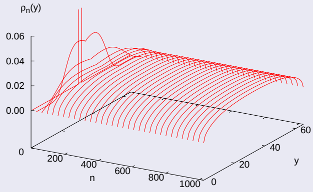
(only 2d shown, 3d similar)

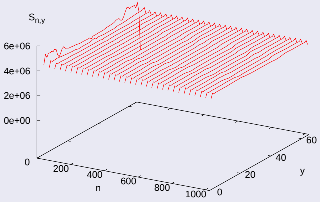


Simulation results: SAW in a strip

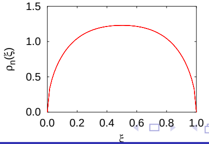
T Prellberg et al, in: Computer Simulation Studies in Condensed Matter Physics XVII, Springer Verlag, 2006

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





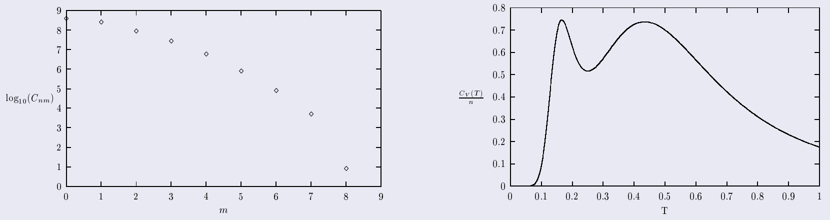
- Scaled endpoint density



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

Extensions

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

- prime example: linear polymers
- but also: permutations (insert $n+1$ into a permutation of $\{1, 2, \ldots, n\}$)

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

- 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)

- An n-step configuration grown has weight

$$W_n = \prod_{i=0}^{n-1} \frac{a_i}{a_{i+1}^-} , \tag{1}$$

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

- Implementing GARM is straightforward
- Computation of atmospheres might be expensive
- Can add pruning/enrichment
- Can extend to flat histogram sampling

Other developments

- add moves that don't change the system size ("neutral" atmosphere)
- 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)

Putting Things in Perspective

As of June 26th,

- PERM (1997): 287 citations
- Multicanonical PERM (2003): 58 citations
- flatPERM (2004): 44 citations
- nPERM (2003): 32 citations
- GARM/flatGARM (2008): 5 citations
- GAS (2009): 5 citation

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This should be compared with e.g.

- Umbrella Sampling (1977): 1288 citations
- Multicanonical Sampling (1992): 868 citations
- Wang-Landau Sampling (2001): 936 citations