ALPS Tutorial
Introduction to Monte Carlo

PSI

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The Monte Carlo trick

$$I = \int_D g(x)dx$$

iid random samples uniformly drawn from *D*

$$\hat{I}_m = \frac{1}{m}\left(g(x^{(1)}) + \cdots + g(x^{(m)})\right)$$

law of the large numbers

$$P\left[\lim_{m\to\infty} |\hat{I}_m - I| = 0\right] = 1$$

The Monte Carlo trick

central limit theorem

$$\lim_{m \to \infty} \mathrm{Cdf}\sqrt{m}\left(\hat{I}_m - I\right) = \mathrm{Cdf}\, N(0, \sigma^2)$$

convergence is

$$\boxed{\mathcal{O}(m^{-1/2})}$$

regardless of the dimensionality of *D*

Importance sampling

$$I = \int_0^\infty g(x) e^{-x} dx$$

draw exponentially distributed random numbers, then

$$\hat{I}_m = \frac{1}{m} \left(g(x^{(1)}) + \cdots + g(x^{(m)}) \right)$$

how?

$u \in [0, 1[$ standard random number generator

$p = -\ln u \quad \Longrightarrow \quad p \in [0, \infty[$

inverse transformation is needed

Importance sampling

Statistical mechanics :

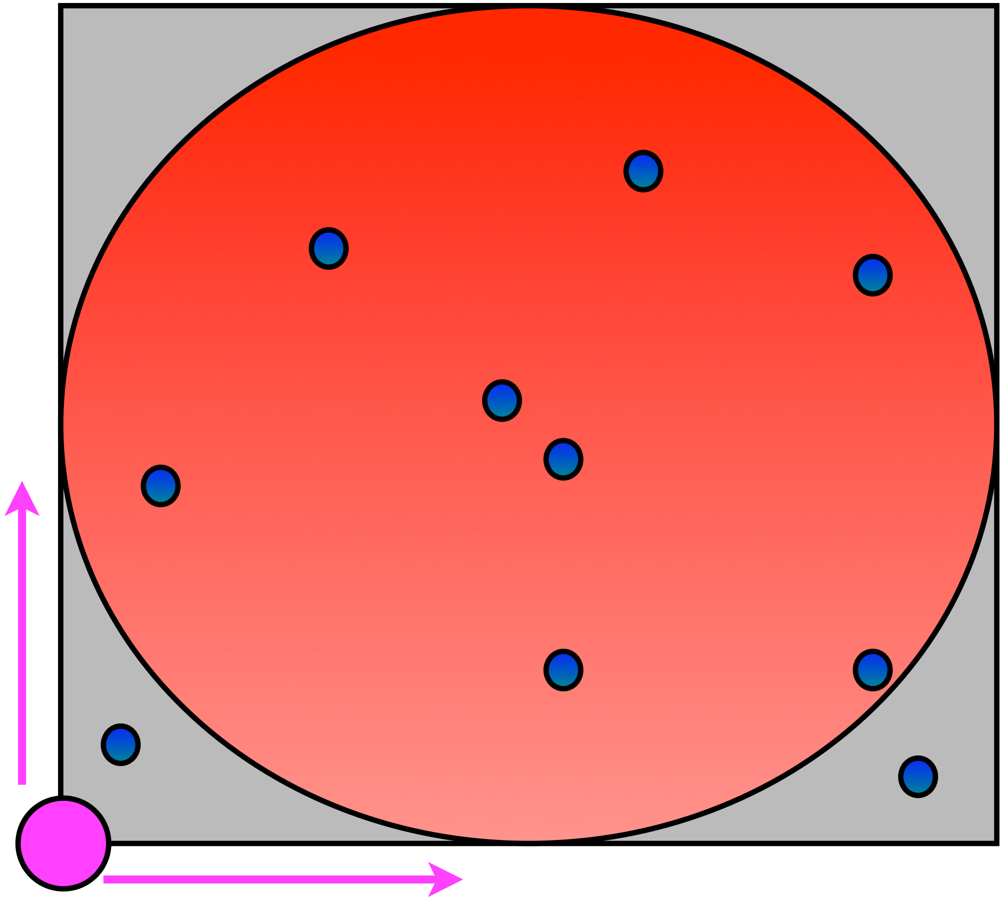
$$\langle Q \rangle = \frac{1}{Z} \mathrm{Tr}\left[Q e^{-\beta H} \right] = \frac{\mathrm{Tr}[Q e^{-\beta H}]}{\mathrm{Tr}[e^{-\beta H}]}$$

unnormalized weights

$$W(x) = e^{-\beta E(x)}$$

how do we get random variables that are distributed according to W(x) ?

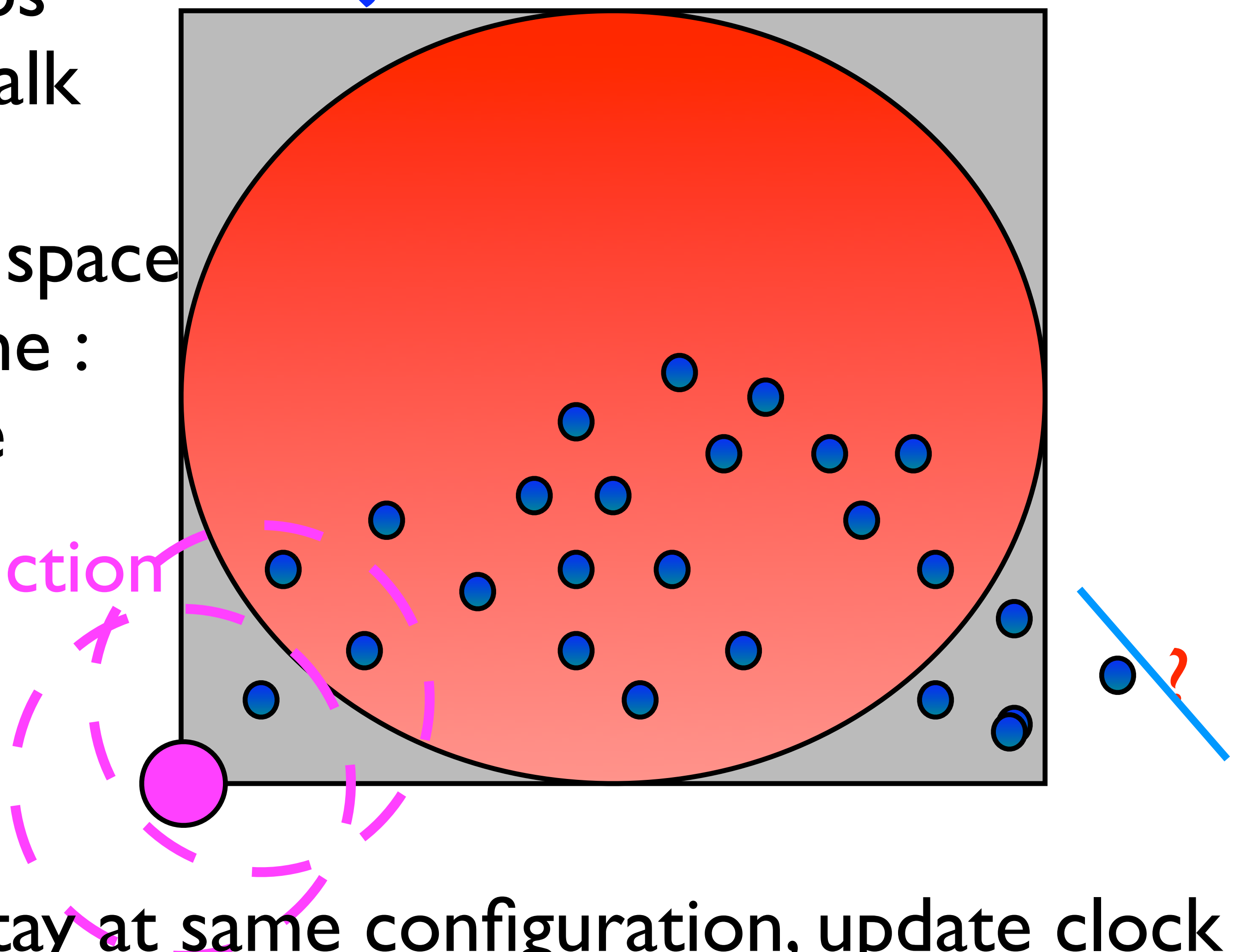
Independent sampling



Known geometry
converges to π/4

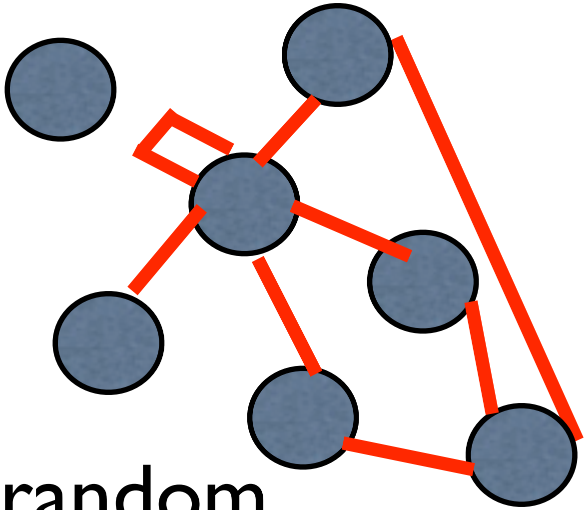
Markov chains and rejections

Small steps random walk through configuration space at each time : measure



Rejection : stay at same configuration, update clock and measure

Markov chain



- A Markov chain is a sequence of random variables $X_1, X_2, X_3, \ldots$ with the property that the future state depends only on the past via the present state.

$$P[X_{n+1} = x | X_n = x_n, \ldots, X_1 = x_1, X_0 = x_0] = P[X_{n+1} = x | X_n = x_n]$$

transition function

$$T(x, y)$$

$$\sum_y T(x, y) = 1$$

conservation of probability

Markov chains

- irreducible
- aperiodic

} convergence to the stationary distribution W

transition kernel has one eigenvalue 1, while all other eigenvalues satisfy

$$|\lambda_j| < 1, j = 2, \ldots N$$

The second largest eigenvalue determines the correlations in the Markov process

Detailed balance

A transition rule *T(x,y)* leaves the target distribution *W(x)* invariant if

$$\sum_x W(x)T(x,y) \sim W(y)$$

This will certainly be the case if detailed balance is fulfilled,

$$W(x)T(x,y) = W(y)T(y,x)$$

Metropolis

we cannot construct a transition kernel T that fulfills detailed balance.

proposal function *P(x,y)*

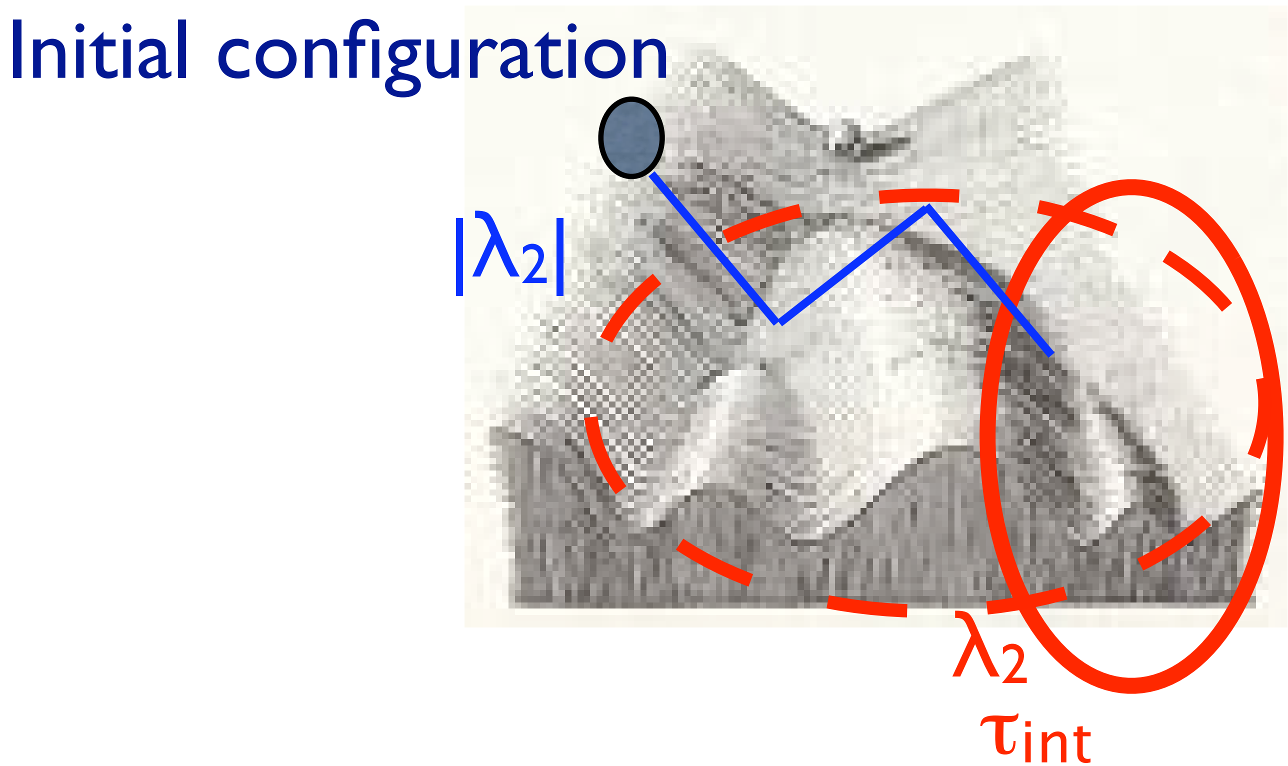
acceptance factor

$$q = \min\left[1, \frac{W(y)P(y,x)}{W(x)P(x,y)}\right]$$

go to the proposed configuration *y* with prob *q*, otherwise stay in *x*

Thermalization

energy landscape

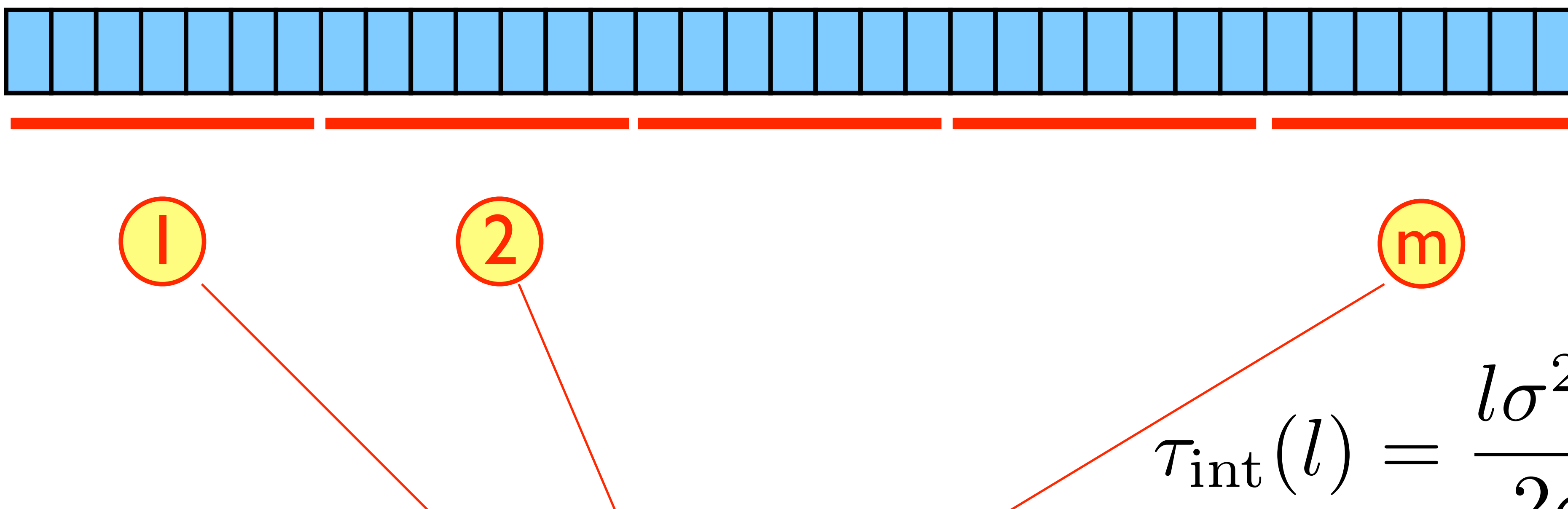


Discard the first 20% of the Markov steps !

Markov Chain should be sufficiently long

Binning analysis

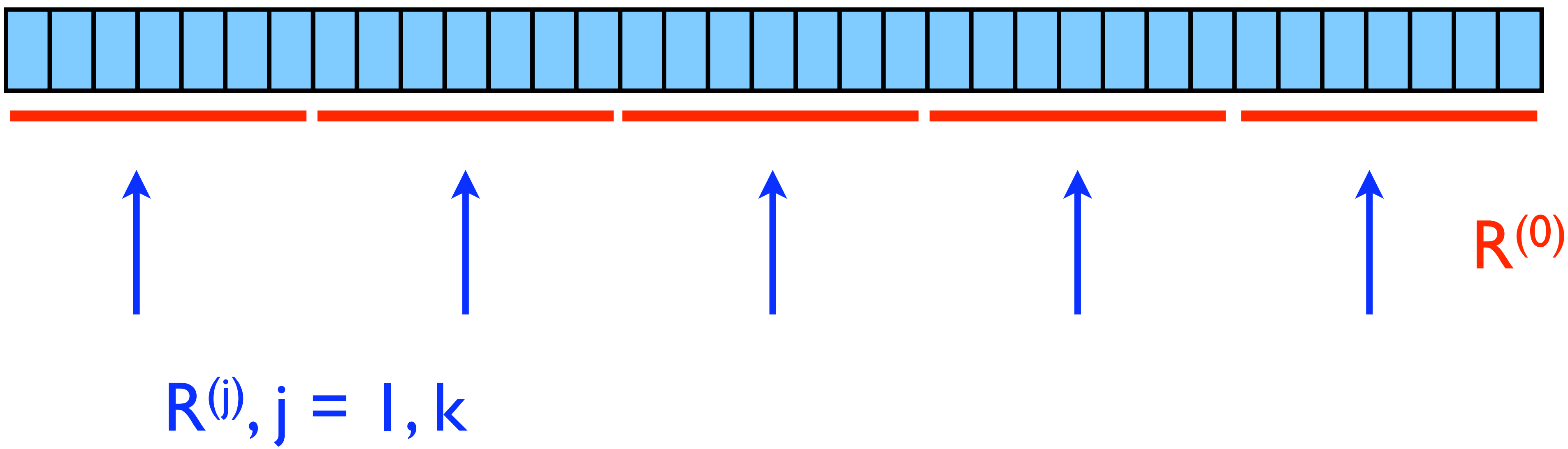
- Markov chain correlates measurements
- if chain is long enough, then the configuration is independent of the initial one



identically and independent

$$\tau_{\mathrm{int}}(l) = \frac{l\sigma^2(l)}{2\sigma^2}$$

Jackknife

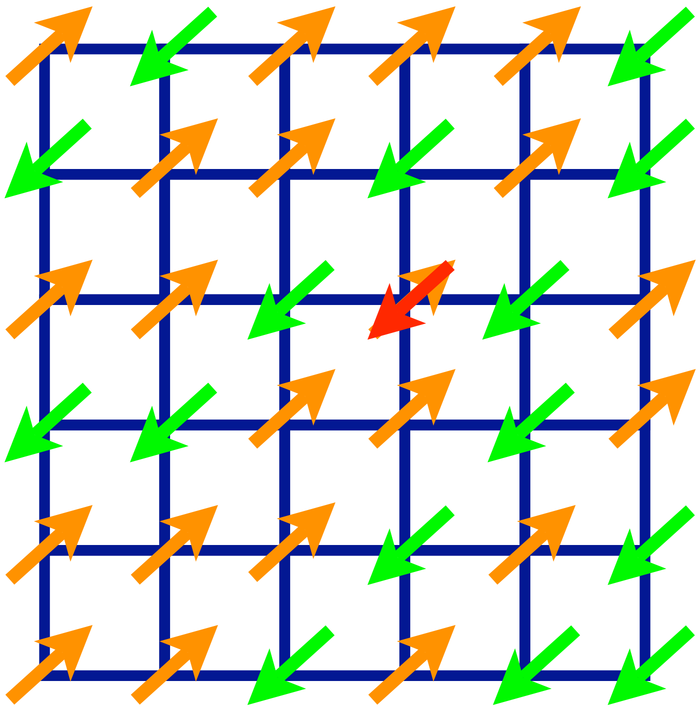


Bias = $(k-1)(R^{av} - R^{(0)})$

$R = R^{(0)}$ - Bias

$$\delta R = \sqrt{k-1}\left(\frac{1}{k}\sum_{j}^{k}(R^{(j)})^2 - (R^{\text{av}})^2\right)^{1/2}$$

Ising model



$$H = -J \sum_{<i,j>} \sigma_i \sigma_j$$

Select random spin

$$P(x,y) = P(y,x) = \frac{1}{L^2}$$

$$\frac{W(y)}{W(x)} = \exp\left(-2\beta J \sigma_i \sum_{<i,j>} \sigma_j \right)$$

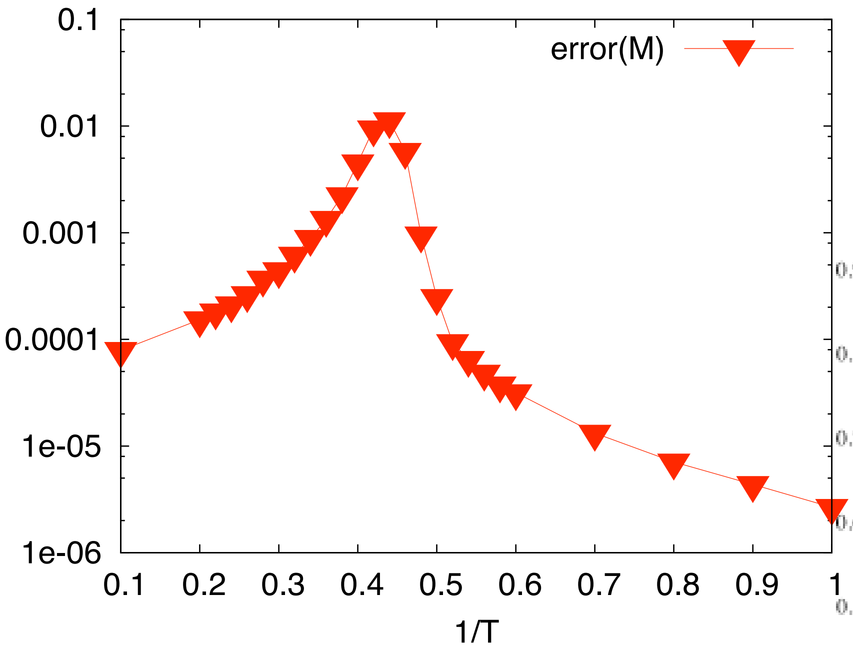
$$W(x)T(x,y) = W(y)T(y,x)$$

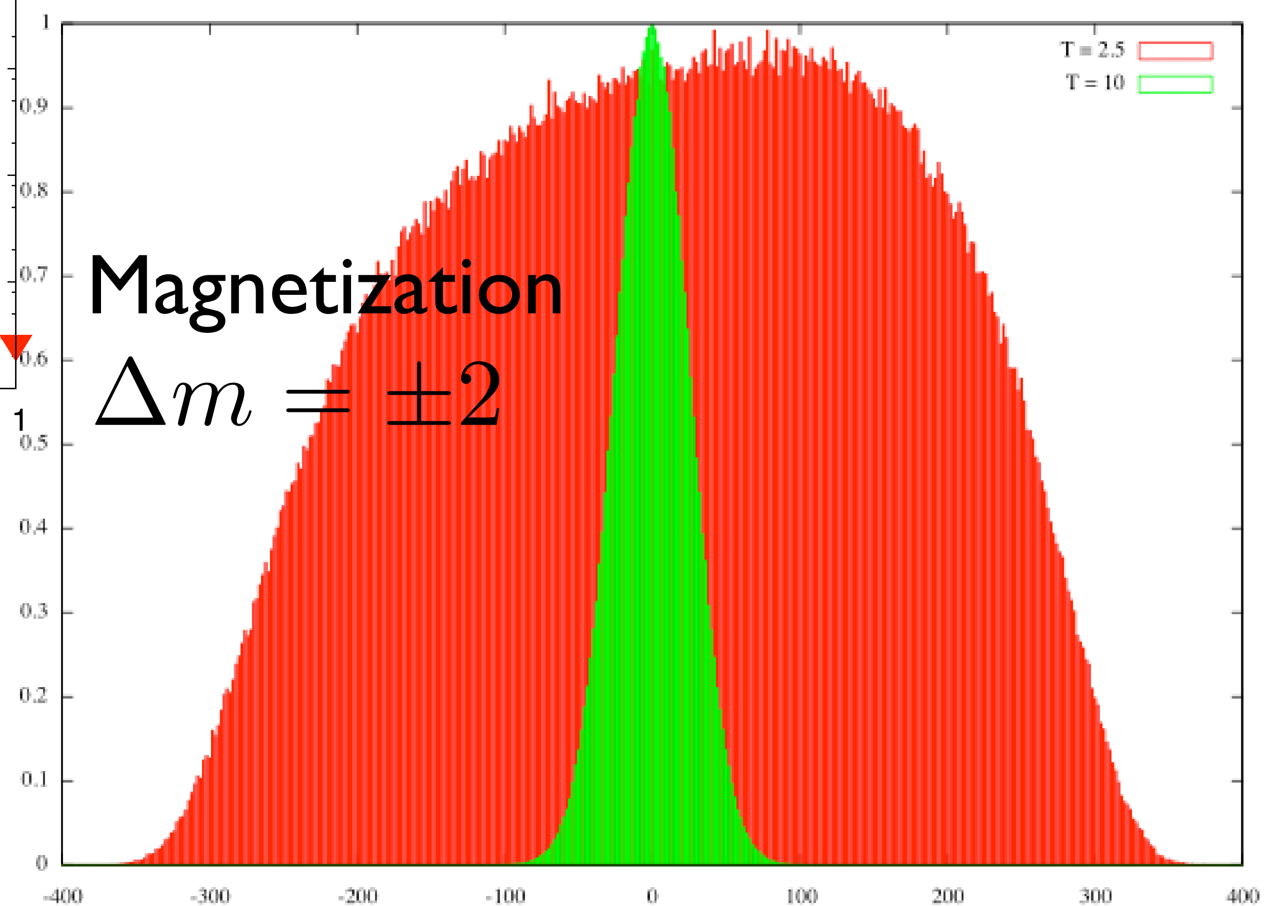
$$q = \min\left[1, \frac{W(y)P(y,x)}{W(x)P(x,y)}\right]$$

$$q = \min\left[1, e^{-2\beta J \sigma_i \sum_{<i,j>} \sigma_j}\right]$$

Critical slowing down

$$T_c = \frac{\ln(1+\sqrt{2})}{2}$$





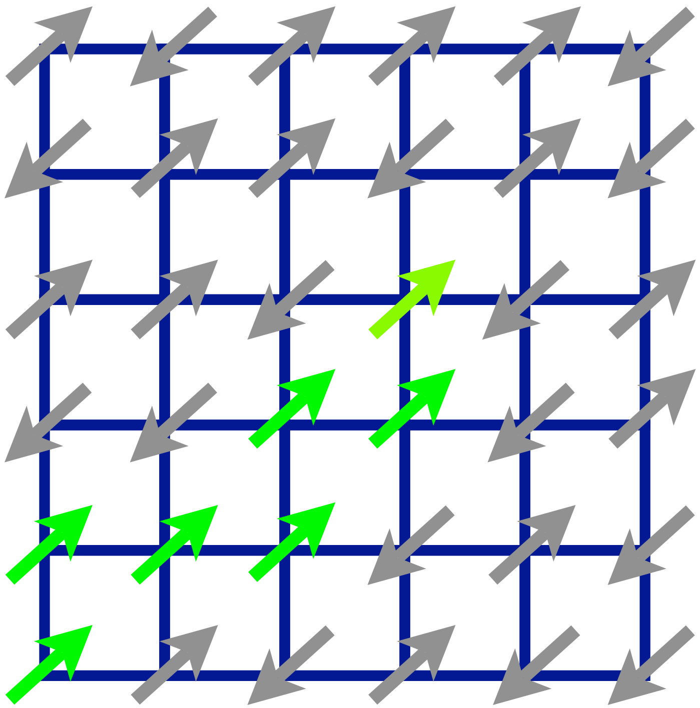
Magnetization

$\Delta m = \pm 2$

divergence of correlation length, critical fluctuations

Magnetization^2	75416	0.649902	0.00429 not converged	10.2	binning

Cluster method (Wolff)



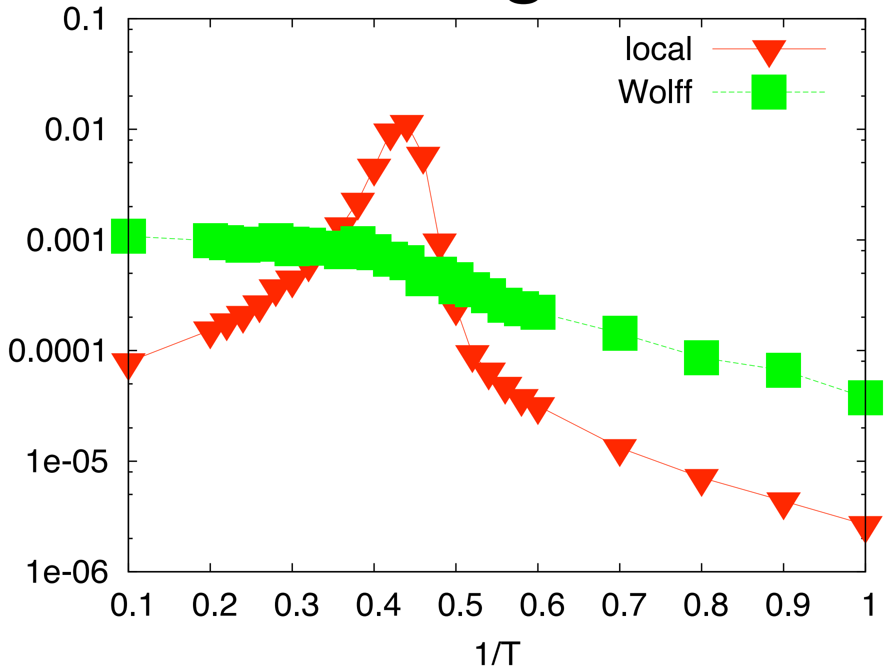
select like spins with probability p

$$p = 1 - \exp[-2\beta]$$

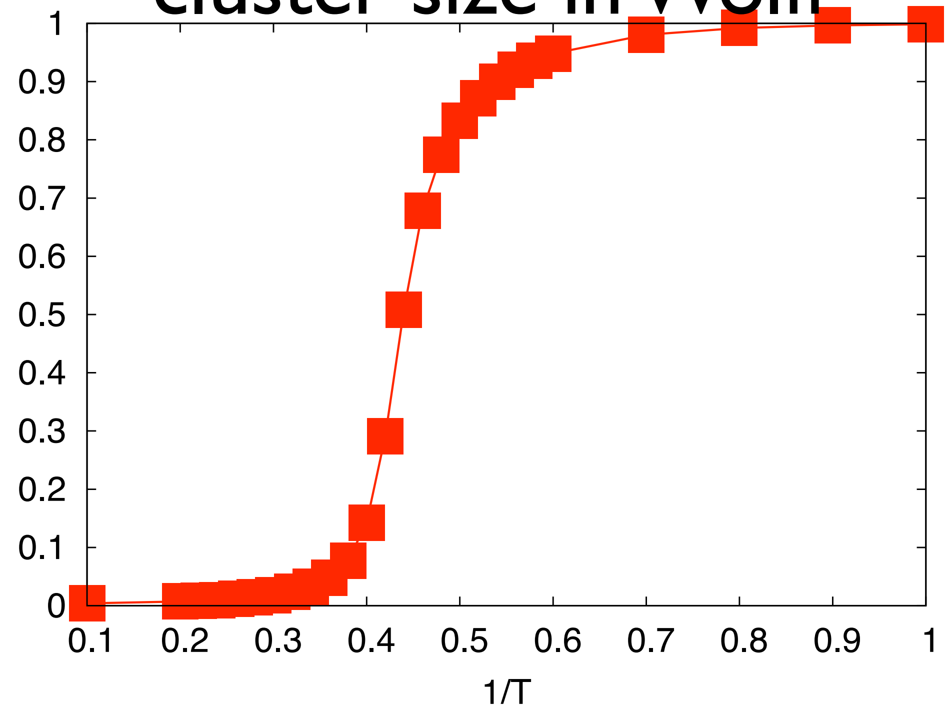
then update always accepted

Phase transition

Error on magnetization



cluster size in Wolff



quantity	functional form	exponent	Ising $d = 2$	Ising $d = 3$
magnetization	$m \propto (T_c - T)^\beta$	β	1/8	0.3258(44)
susceptibility	$\chi \propto \|T - T_c\|^{-\gamma}$	γ	7/4	1.2390(25)
correlation length	$\xi \propto \|T - T_c\|^{-\nu}$	ν	1	0.6294(2)
specific heat	$C(T) \propto \|T - T_c\|^{-\alpha}$	α	0	
inverse critical temp.		$1/T_c$	$\frac{1}{2}\ln(1+\sqrt{2})$	0.221657(2)

Thanks !