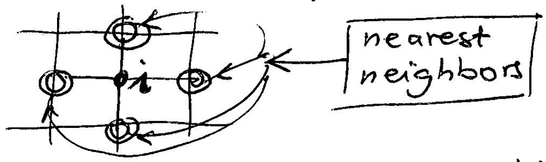
As in the Metropolis algorithm, we choose a spin σ_i and propose an update for it

[Ising Model: $H = -\sum_{<ij>} \sigma_i \sigma_j$, $\sigma_1 = \pm 1$]

We consider the conditional probability of σ_i

all contributions that do not depend on i

$$H = H_0 - \sum_j \sigma_1 \sigma_j$$



IN 2D this sum goes over the 4 nearest neighbors

Corrections : Change H0 - sigma1 V into H0+ sigma1 V and add a sign in the definition of V

$$= H_0 - \sigma_1 V \qquad V = \sum_j \sigma_j \text{ (sum over nearest neighbors)}$$

$$\pi_{cond}(\sigma_1) = \frac{1}{Z} e^{-\beta H_0} e^{-\beta V \sigma_i} = a e^{-\beta V \sigma_i}$$

The normalization constant a follows from

$$\pi_{cond}(+1) + \pi_{cond}(-1) = 1 \implies a = \frac{1}{e^{\beta V} + e^{-\beta V}}$$

PRACTICAL IMPLEMENTATION

(a) select i (sequentially or randomly)

(b) if (RAN( ).less than $a e^{-\beta V}$)

$\sigma_1 = +1$ $\qquad (\sigma_1 = +1 \text{ prob } a e^{-\beta V})$

else

$\sigma_1 = -1$ $\qquad (\sigma_1 = -1 \text{ prob } a e^{\beta V})$

end if

HEAT BATH AS A METROPOLIS ALGORITHM

In the Metropolis algorithm, we fix the acceptance matrix solving the equation

$$\frac{A_{xy}}{A_{yx}} = R_{xy}$$

The optimal Metropolis choice is $A_{xy} = \min(1, R_{xy})$

There are other solutions.

Now we show that

$$A_{xy} = \frac{R_{xy}}{1+R_{xy}}$$

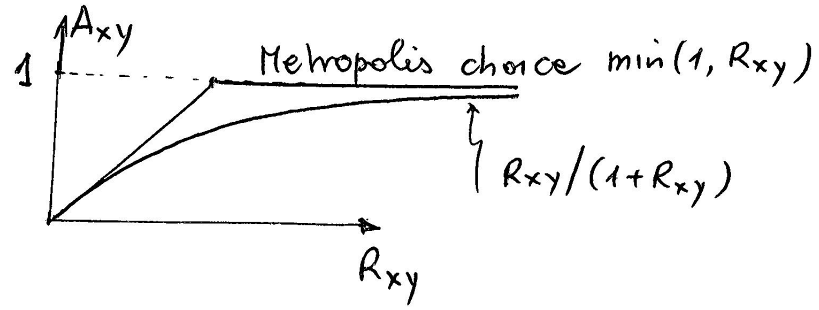
is a solution

Now $$A_{yx} = \frac{R_{yx}}{1+R_{yx}} = \frac{\frac{1}{R_{xy}}}{1+\frac{1}{R_{xy}}} = \frac{1}{1+R_{xy}} \qquad \left[R_{xy} = \frac{1}{R_{yx}}\right]$$

Therefore

$$\frac{A_{xy}}{A_{yx}} = \frac{R_{xy}}{1+R_{xy}} \cdot (1+R_{xy}) = R_{xy} \qquad \text{OK}$$

Less efficient



PROPOSAL: Same as in the standard Metropolis algo.

$$\begin{cases} \text{if } \sigma_1 = 1 & \text{we propose } \sigma_1 = -1 \\ \text{if } \sigma_1 = -1 & \text{we propose } \sigma_1 = 1 \end{cases} \qquad \underset{\sigma_1=+1}{P^{(0)}_{+-}} = \underset{\sigma_1=-1}{P^{(0)}_{-+}} = 1$$

The factor R is given by

$$R_{+-} = \frac{\pi_-}{\pi_+} = \frac{a e^{\beta V}}{a e^{-\beta V}} = e^{2\beta V} \qquad R_{-+} = \frac{1}{R_{+-}} = e^{-2\beta V}$$

Acceptance

$$A(\sigma_1 = 1 \to \sigma_1 = -1) = A_{+-} = \frac{R_{+-}}{1 + R_{+-}} = \frac{e^{2\beta V}}{1 + e^{2\beta V}} = \frac{e^{\beta V}}{e^{\beta V} + e^{-\beta V}}$$

$$A(\sigma_1 = -1 \to \sigma_1 = +1) = A_{-+} = \frac{R_{-+}}{1 + R_{-+}} = \frac{e^{-2\beta V}}{1 + e^{-2\beta V}} = \frac{e^{-\beta V}}{e^{\beta V} + e^{-\beta V}}$$

The transition matrix

$$P(\sigma_1 = 1 \to \sigma_1 = -1) = P^{(0)}_{+-} A_{+-} = a e^{\beta V}$$

$$P(\sigma_1 = 1 \to \sigma_1 = +1) = 1 - P(\sigma_1 = 1 \to \sigma_1 = -1) = a e^{-\beta V}$$

SAME AS IN THE HEATBATH ALGO.

$$P(\sigma_1 = -1 \to \sigma_1 = +1) = P^{(0)}_{-+} A_{-+} = a e^{-\beta V}$$

$$P(\sigma_1 = -1 \to \sigma_1 = -1) = 1 - P(\sigma_1 = -1 \to \sigma_1 = +1) = a e^{\beta V}$$

SAME AS IN THE HEATBATH ALGO.