while $SIZES(L) < 0$: $L = -SIZES(L)$

write L to the LABEL lattice, $SIZES(L) += 1$

- both are occupied:

find both root labels, take the smaller and unify them

($L_1 < L_2$: $SIZES(L_1) += SIZES(L_2) + 1$

$SIZES(L_2) = -L_1$)

at the end the SIZES array has what we need.

~~full label~~ : TRICK: do this alg as occupations are generated.

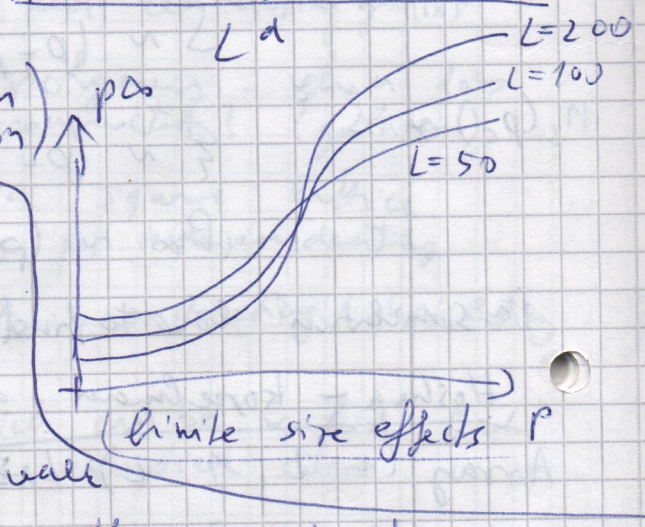
. we can forget old rows. (we need L^{d-1} storage)

[in $d=2$ $p = \frac{1}{2}$ for triangular latt

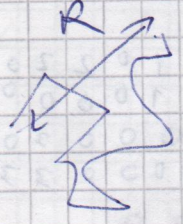
$p = 0.5927$ square latt) $\nu = 4/3$ $\beta = \frac{5}{36}$

for finite lattice e.g. $P_\infty = \frac{\text{points in largest cluster}}{L^d}$

(generalizations bond percolation directed percolation)



Random walks Conformation of a polymer chain



$R \sim N^\nu$

simplest model: Random walk

$\rightarrow R \sim t^{1/2}$ disagrees with experiment.

no backtrack RW : do not immediately turn back

SAW self avoiding random walk : do not go to a site already visited (monomers repulse)

What should be the weight of a Random walk?

RW : all walks of length N are equally probable

SAW : " " as long as they are SAWs

⇒ generate RWs, throw away if they intersect
works for small N, otherwise most RWs are thrown away (attrition problem)

Rebtation algorithm:

1. Assume we ha a walk.
2. delete one point from a random end
3. add one point to a random end with random direction. accept the new walk if it is SAW
otherwise use old as new config.

Pivot algorithm Use lattice symmetries

$\nu = 3/4$ $d=2$

$\nu = 0.59\ldots$ $d=3$

$\nu = 1/2$ $d=4$

Biased sampling.

Check how many steps are available (no backtrace)

$$W = \prod_{i=1}^{N} \frac{l_i}{(2d-1)}$$ ← number of steps possible at step i

Generalization: potential between monomers.
now different walks have different weights.

Importance Sampling.

Usual question: $$\langle F \rangle = \frac{1}{Z} \int F(p,q)\, e^{-\beta H(p,q)}\, dp^n\, dq^n$$

$e^{-\beta H(p,q)} \approx 0$ for most configurations

$$\langle F \rangle = \int F(E) \cdot \rho(E) \cdot e^{-\beta E}\, dE$$

$\rho(E) \cdot e^{-\beta(E)}$ is sharply peaked

uniform random configurations have too little weight ($\rho \approx 0$) or too large energy $\rho(E)\, e^{-\beta E} \approx 0$

if we sample with prob. $e^{-\beta H(p,q)}$

$$\langle F \rangle = \frac{1}{N} \sum F(p_i, q_i)$$

Metropolis algorithm

Markov chain

i – computer time

$\phi_i \to \phi_{i+1} \to \phi_{i+2} \dots$

prob. to go from ϕ to ϕ' = $T(\phi'|\phi)$

T does not depend on i, only on ϕ not older ϕs $\Rightarrow$

$\Rightarrow$ Markov process

$P(Q)$ = prob. of state Q

$$\sum_{\phi'} T(\phi'|\phi) = 1$$

Master eq.: $\frac{\partial P(Q,t)}{\partial t} = \sum_{Q'} W(Q \leftarrow Q') P(Q') - \sum_{Q'} W(Q' \leftarrow Q) P(Q)$

discretised

$$P_{i+1}(\phi) = \sum_{\phi} T(\phi|\phi') P_i(\phi') \quad \cancel{T(\phi'|\phi) P_i(\phi)}$$

going in — going out

$P_j^{(n+1)} = T_{jk} P_k^{(n)}$

$P_j^{(n+1)} - P_j^{(n)} = T_{jk} P_k^{(n)} - P_j^{(n)} =$

in equilibrium $\pi(\phi)$ $= \sum_k T_{jk} P_k^{(n)} - \sum_k T_{kj} P_j^{(n)}$

Balance equation no source or sink

$$\pi(\phi) = \sum_{\phi'} T(\phi|\phi') \pi(\phi') = \sum_{\phi'} T(\phi'|\phi) \pi(\phi)$$

(going in) (going out)

in Matrix notation

$$T_{ik} \Phi_k = \Phi_i$$

eigenvector with e.v. = 1

$\forall_i \forall_j \exists N \; (T^N)_{ij} > 0$ irred

$\forall_i \forall_j \; T_{ij} > 0$ aperiodic

$\forall_i \forall N \; (T^N)_{ii} > 0$

Let's choose $T(\phi|\phi')$ such that we have

detailed balance

$$T(\phi'|\phi)\, \pi(\phi) = T(\phi|\phi')\, \pi(\phi')$$

current is the same in both directions $T_{ij} \pi_j = T_{ji} \pi_i$

consider the evolution of $P^{(1)} \to P^{(2)} \to$

does it converge to π?

$$\sigma_N = \sum_i |P_i^{(N)} - \pi_i|$$

$$\sigma_{N+1} = \sum_i |T_{ij} P_j^{(N)} - \pi_i| = \sum_i |T_{ij} P_j^{(N)} - T_{ji} \pi_i| =$$

$$= \sum_i \left| \sum_j \left(T_{ij} P_j^{(N)} - T_{ij} \pi_j \right) \right| \le \sum_{i,j} T_{ij} |P_j^{(N)} - \pi_j| = \sigma_N$$

$\sum_i P_j^{(N)} - \pi_j = 0$, $T_{ij} > 0$ $\Rightarrow$ equality only if $\sigma_N = 0$

$\Rightarrow$ convergence to unique eq. π

Metropolis alg.

starting from state ϕ_0. After $n-1$ steps, do

1. proposal $T_0(\phi' | \phi_{n-1})$
2. Acceptance probability $T_A(\phi' | \phi_{n-1})$

if accepted $\phi_n = \phi'$

else $\phi_n = \phi_{n-1}$

To satisfy detailed balance, we must have

$$T_0(\phi|\phi') \cdot T_A(\phi|\phi') \cdot \pi(\phi') = T_0(\phi'|\phi)\, T_A(\phi'|\phi) \cdot \pi(\phi)$$

$$\frac{T_0(\phi|\phi')\, T_A(\phi|\phi')}{T_0(\phi'|\phi)\, T_A(\phi'|\phi)} = \frac{\pi(\phi)}{\pi(\phi')}$$

$$\frac{T_A(\phi|\phi')}{T_A(\phi'|\phi)} = \frac{\pi(\phi)}{\pi(\phi')} \cdot \frac{T_0(\phi'|\phi)}{T_0(\phi|\phi')} = F(\phi|\phi')$$

we can choose e.g. $T_A^{(\phi\phi')} = \begin{cases} F(\phi|\phi') & \text{if } F(\phi|\phi') < 1 \\ 1 & \text{otherwise} \end{cases}$

or $T_A(\phi|\phi') = \dfrac{F}{1+F}$

usually $T_0(\phi|\phi') = T_0(\phi'|\phi)$ reversibility of proposal

$$\pi(\phi) = e^{-S[\phi]}$$

$$\frac{\pi(\phi)}{\pi(\phi')} = e^{-(S(\phi)-S(\phi'))} = e^{-\Delta S}$$

in this case acceptance prob $= \begin{cases} e^{-\Delta S} & \text{if } \Delta S > 0 \\ 1 & \text{if } \Delta S < 0 \end{cases}$

$T_0(\phi|\phi') = ?$ should be optimized

change too big $\Rightarrow$ acceptance small

change too small $\Rightarrow$ conf. space exploration is slow

e.g. for Ising model

local change $s_i \to -s_i$ OK for most cases except near critical phase transition

cluster alg: change many spins at once