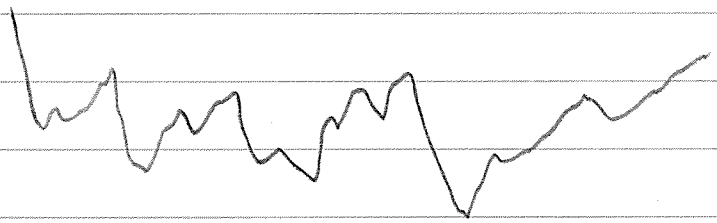
## Simple algorithms for difficult problems

Ex Spin glass $H = \sum_{\langle ij \rangle} J_{ij} s_i s_j$

where $J_{ij}$ can be both positive and negative,
e.g., $J_{ij} \sim N(0, \sigma^2)$ normal distribution

At low T the spins will freeze into a random glass configuration, with a lot of frustrated bonds.

Very rugged energy landscape



The simulation easily gets trapped in local minima
⇒ Finding the ground state is a hard optimization problem

## Simulated annealing

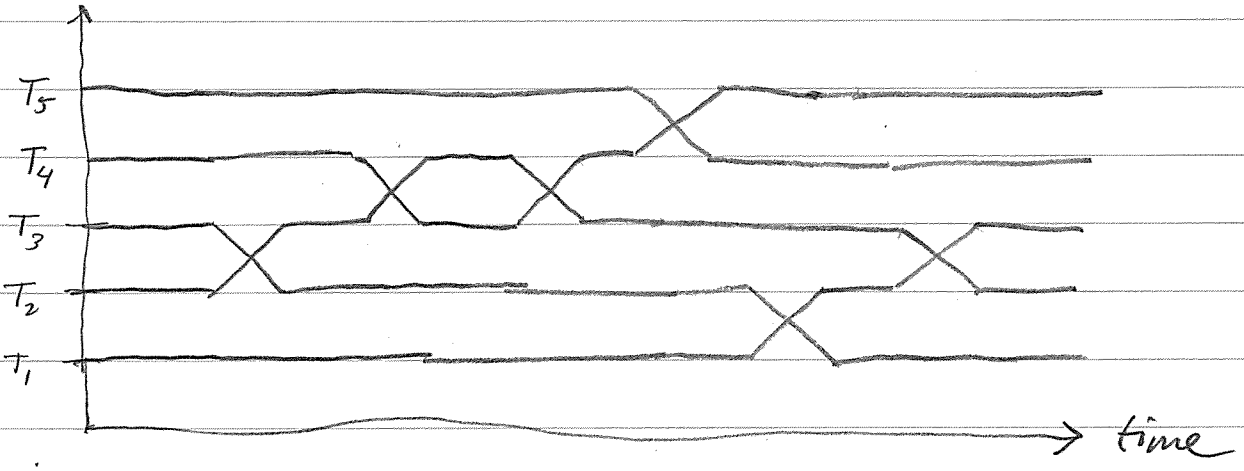
Run a MCMC simulation starting at high temperature, where energy barriers are easily crossed, and then slowly cool it to zero temperature.

If the rate of cooling is slow enough it may be possible to reach the ground state or at least very deep minima with high probability.

# Parallel tempering a.k.a. (Replica) Exchange MC

Run $M$ simulations at different temperatures $T_1 < T_2 < \dots < T_M$ in parallel.

Occationally swap two systems with neighbouring $T$.




Each replica will essentially carry out a random walk in temperature and randomly heat up and cool down and thereby get many opportunities to explore local minima and escape traps.

The partition function of the whole <u>generalized ensemble</u> of systems is simply a product

$$Z_{PT} = \prod_{m=1}^{M} Z_{\beta_m} = \sum_{\{x_m\}} \prod_{m=1}^{M} e^{-\beta_m E(x_m)}$$

Metropolis acceptance probability for a swap $\beta_m \leftrightarrow \beta_{m+1}$:
$A = \min(1, e^{-\Delta})$

$$\Delta = (\beta_{m+1} - \beta_m) E(x_m) + (\beta_m - \beta_{m+1}) E(x_{m+1}) =$$
$$= -\Delta\beta \cdot \Delta E \quad , \quad \Delta\beta = \beta_{m+1} - \beta_m \, , \quad \Delta E = E(x_{m+1}) - E(x_m)$$

The temperature spacing must be small enough that exchanges are accepted with reasonable probability.
⇒ Need that the canonical distributions $\pi_\beta(x)$ overlap for neighbouring temperatures.
One possibility is to fine tune the $\beta_m$ to get a roughly constant acceptance probability.

Note that the samples collected at a given $\beta_m$ will follow the usual canonical $\pi_{\beta_m}(\cdot)$ so we can estimate any canonical expectation $\langle A \rangle_{\beta_m}$.

Even better, we can use multihistogram reweighting - WHAM (or MBAR).

Another generalized ensemble is the <u>Multicanonical ensemble</u>. Very useful at 1st order phase transitions.

Recall that in a canonical ensemble
$\pi(x) = \frac{1}{Z} e^{-\beta E(x)}$,
and the marginal distribution for the energy $E$ is
$\pi(E) = \frac{1}{Z} \Omega(E) e^{-\beta E}$, where $\Omega(E)$ is the density of states.
= # states with energy $E$.

In a Multicanonical ensemble the target distribution is instead
$$\pi(x) \propto \frac{1}{\Omega(E(x))} \Rightarrow \pi(E) \propto \frac{\Omega(E)}{\Omega(E)} = \text{const.}$$
⇒ All energies sampled with equal prob.

# Wang-Landau method

Since we don't know $\Omega(E)$ from the start we begin with a guess for it, e.g. $\Omega(E) = 1$

Run a Metropolis algorithm as usual but with a different acceptance probability

$$A(X \leftarrow X') = \min\left(1, \frac{\Omega(E)}{\Omega(E')}\right), \quad \text{where } E = E(x),\ E' = E(x')$$

Each time an energy level $E$ is visited we update the DOS at that energy:

$$\Omega(E) \leftarrow \Omega(E) \cdot f$$

where $f > 1$ is a certain modification factor.
At the start of the simulation $f$ is set to $f_0 = e^1$ typically.

Note that $\pi(x) \propto \frac{1}{\Omega(E)}$ so each multiplication of $\Omega(E)$ by $f$ will decrease somewhat the probability to visit that energy.

During the simulation a histogram $H(E)$ of visited energies is collected. When the histogram is sufficiently flat, as defined by some flatness-criterion, the modification factor is decreased: $f_{n+1} \leftarrow \sqrt{f_n}$
and the histogram is reset to zero,
and the simulation continues with its refined $f_{n+1}$.

Eventually $\Omega(E)$ will be an approximation to the true DOS and can be used to calculate canonical expectations by reweighting.