The Monte Carlo technique

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Basic idea: Solve problems by drawing random numbers
Example: Determination of π (problem set 1, exercise 2)

In **statistical physics**, we often need to determine **expectation values** of an observable O for a given system in a given statistical ensemble.

Problem: 1. Oftentimes, the number of all possible states is astronomically large, even for small systems
→ in most cases **complete enumeration is not an option**

Example: 3d lattice with 10 potential positions along each axis, 10 particles. How many different states exist?
Non-interacting particles: $1000*\ldots*1000=10^{30}$
Interacting particles: $2.6*10^{23}$

2. **Random sampling is** often **not an option either**, because many states only yield a negligible contribution to the average

Example: If the particles above are attractive, they like to form a cluster at low temperatures
→ putting in particles at random is very inefficient

Solution: Generate only states which contribute significantly to the mean.

Importance sampling

In the following we will discuss the concept of importance sampling in the context of statistical physics. In particular, we will focus on the canonical (NVT) ensemble. Other ensembles will be considered in the Advanced Monte Carlo section.

In the canonical ensemble the probability to obtain a given state S_i is given by

$$P_i = \frac{e^{-\beta E_i}}{Z}$$ "Botzmann-distributed"

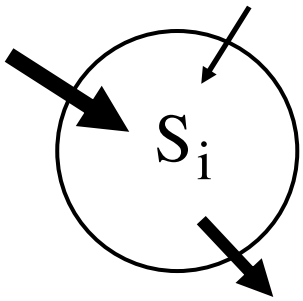
P_i: probability to find system in state S_i
E_i: energy of state S_i
Z: partition sum

Basic idea:

We consider the probability flows in and out of particular states.

Flow out of state S_i: $\sum_j P_i(t) W_{ij}$

Flow into state S_i: $\sum_j P_j(t) W_{ji}$



$P_i(t)$: probability that system resides in state S_i at time t.
W_{ij}: probability that system jumps from state S_i to state S_j

In equilibrium, all states are in equilibrium with each other, i.e., the **total flow out of a state is equal to the total flow into that state**:

$$\sum_j P_i(t) W_{ij} = \sum_j P_j(t) W_{ji}$$ **MASTER EQUATION**

This equation is fulfilled by any means, if the following (stricter) equation is fulfilled for all i,j:

$$P_i(t) W_{ij} = P_j(t) W_{ji}$$ **DETAILED BALANCE**

Vice versa, a system which is currently out of equilibrium will move towards equilibrium if detailed balance is enforced.

Task: Choose W_{ij} such that detailed balance is fulfilled, i.e., $\frac{W_{ij}}{W_{ji}} = e^{-\beta(E_j - E_i)}$

The Metropolis Criterion (Metropolis et al, J.Chem.Phys. 21, 1087, 1953)

The following rule enforces detailed balance:

$W_{ij}=\exp(-\beta\Delta E)$, if $\Delta E=E_j-E_i>0$ and $W_{ij}=1$, if $\Delta E<0$, i.e.,

Monte Carlo moves which lower the energy of the system are always accepted ($W_{ij}=1$). If the energy of the system increases, the move is accepted with probability $\exp(-\beta\Delta E)$, i.e., the higher the energy becomes, the lower the acceptance.

Proof: $\Delta E<0$ $\frac{W_{ij}}{W_{ji}} = \frac{1}{e^{\beta(E_j - E_i)}}$

Keep in mind that for the reverse move from S_j to S_i, "ΔE">0 and indices are interchanged. $\Delta E>0$: homework