Block 10 (Donnerstag 29.2.2024)

# 11 Monte Carlo Simulations

VIDEO: `video08b_markov_ketten_r`

## 11.1 Markov Chains

Given; sytsem with (a finite number of) states $\underline{y} = \underline{y}_1, \underline{y}_2, \ldots, \underline{y}_K$ and probabilities $P(\underline{y})$.
Typical:$K$ exponentially large in number $N$ of particles and $P(\underline{y})$ significant only for an exponentially small fraction of states ($\sum_{\text{significant }\underline{y}} 1/K \to 0$ and $\sum_{\text{significant }\underline{y}} P(\underline{y}) \to 1$)
Example: Boltzmann distribution
Target: Estimation of expectation values of obervables $A(\underline{y})$

$$\langle A \rangle := \sum_{\underline{y}} A(\underline{y}) P(\underline{y}) \tag{52}$$

Assumption: $K$ very large $\to$ impossible to enumerate all states.

*Simple Sampling*:

Generate $M$ states $\{\underline{y}^i\}$ $(i = 1, \ldots, M)$ randomly, with uniform probability. Then:

$$\langle A \rangle \approx \overline{A}^{(1)} := \sum_{\underline{y}^i} A(\underline{y}^i) P(\underline{y}^i) / \sum_{\underline{y}^i} P(\underline{y}^i)$$

Drawback: for almost all states $P(\underline{y}^i)$ is exponentially small $\to$ $\overline{A}^{(1)}$ not accurate.
*Importance Sampling*:

Better: generate $M$ configurations $\underline{y}^i$ according to $P(\underline{y}^i)$. (generate *most important states* more often), then:

$$\langle A \rangle \approx \overline{A}^{(2)} := \sum_{\underline{y}^i} A(\underline{y}^i)/M \tag{53}$$

But: usually no algorithm to generate $y^i$ directly according to $P(\underline{y}^i)$ (distribution function cannot be obtained or inverted).

$\rightarrow$
Baisc idea: states $\underline{y}^i$ are *not* generated independently but by a *probabilistic dynamics* of states $\underline{y}(t)$ at discrete times $t = 0, 1, 2, \ldots$: $\underline{y}(0) \rightarrow \underline{y}(1) \rightarrow \underline{y}(2) \rightarrow \ldots$.

Assumption: states $\underline{y}(t+1)$ depend only on random numbers and on $\underline{y}(t)$. $\{\underline{y}(t)|t = 0, 1, 2, \ldots\}$ is called a *Markov chain*.
Description of transitions $\underline{y}(t) \rightarrow \underline{y}(t+1)$ by $W_{\underline{y}\underline{z}} = W(\underline{y} \rightarrow \underline{z})$ = probability to move from state $\underline{y}$ (at time $t$) to state $\underline{z}$ (at time $t+1$), where $W_{\underline{y}\underline{z}}$ does not depend on time.

[Activator]

Which properties has $W_{\underline{y}\underline{z}}$?

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The state space plus the transition probabilities is called a *Markov process*.

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Example: Two state system

Two states A,B and transition probabilities $W_{AA} = 0.6$, $W_{AB} = 0.4$, $W_{BA} = 0.1$, $W_{BB} = 0.9$.

Assumption: One generates $N = 100$ Markov chains, which all start in $A$: $N(A/B, t)$ = number of chains which are in state $A/B$, at time step $t$. Let $N(A, 0) = 100$ and $N(B, 0) = 0$. How could the dynamics look like?

For (about) average values Mittelwerte: $N(A, 0)W_{AB} = 100 \times 0.4 = 40$ chains move from $A \rightarrow B$, while no transitions happen $B \rightarrow A$ at $t = 0$. An so on. Evolution:

$$t = 0: \quad \boxed{\text{N(A)=100}} \; \overset{0}{\longleftarrow} \underset{\longrightarrow}{40} \; \boxed{\text{N(B)=0}}$$

$$t = 1: \quad \boxed{\text{N(A)=60}} \; \overset{4}{\longleftarrow} \underset{\longrightarrow}{24} \; \boxed{\text{N(B)=40}}$$

$$t = 2: \quad \boxed{\text{N(A)=40}} \; \overset{6}{\longleftarrow} \underset{\longrightarrow}{16} \; \boxed{\text{N(B)=60}}$$

$$t = 3: \quad \boxed{\text{N(A)=30}} \begin{array}{c} \xleftarrow{7} \\ \xrightarrow{12} \end{array} \boxed{\text{N(B)=70}}$$

$$t = 4: \quad \boxed{\text{N(A)=25}} \begin{array}{c} \xleftarrow{8} \\ \xrightarrow{10} \end{array} \boxed{\text{N(B)=75}}$$

$$t = 5: \quad \boxed{\text{N(A)=23}} \begin{array}{c} \xleftarrow{8} \\ \xrightarrow{9} \end{array} \boxed{\text{N(B)=77}}$$

$$t = 6: \quad \boxed{\text{N(A)=22}} \begin{array}{c} \xleftarrow{8} \\ \xrightarrow{9} \end{array} \boxed{\text{N(B)=78}}$$

$$t = 7: \quad \boxed{\text{N(A)=21}} \begin{array}{c} \xleftarrow{8} \\ \xrightarrow{8} \end{array} \boxed{\text{N(B)=79}}$$

From now on about $N(A,t)W_{AB} = N(B,t)W_{BA}$. The transfer between states balances $\rightarrow$ $N(A/B,t)$ =const, *stationary state* □

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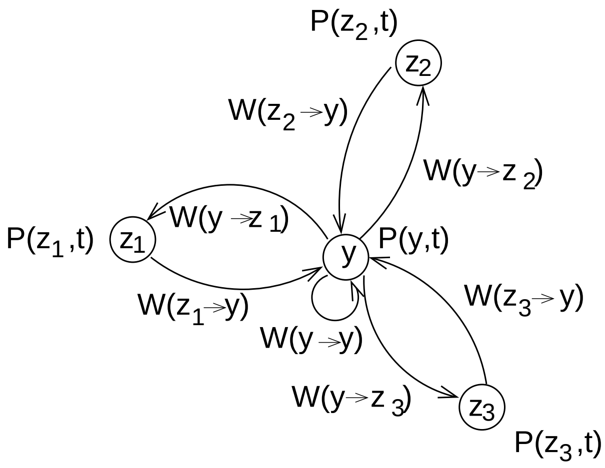
General:
Let $P(\underline{y},t) = \langle N(\underline{y},t)/N \rangle$ the probability that system at time $t$ is in state $\underline{y}(t) = \underline{y}$. Balance for state $\underline{y}$:




Therefore ("Master Equation"):

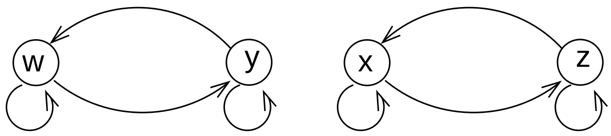
$$\Delta P(\underline{y},t) := P(\underline{y},t+1) - P(\underline{y},t) = \sum_{\underline{z}} W_{\underline{z}\underline{y}} P(\underline{z},t) - \sum_{\underline{z}} W_{\underline{y}\underline{z}} P(\underline{y},t) \quad \forall \underline{y} \quad (54)$$

Under specific conditions (in particular if there is only one eigen value $\lambda = 1$ of matrix $\hat{W}$ ($\hat{W}_{\underline{y}\underline{z}} = W_{\underline{y}\underline{z}} - \delta_{\underline{y}\underline{z}} \sum_{z'} W_{\underline{y}\underline{z}'}$), see L. Reichel, 1998 [7]), the probability distribution $\to$ *stationary* (time-independent) distribution.

$$P_{ST}(\underline{y}) := \lim_{t\to\infty} P(\underline{y}, t)$$

Independent of given initial state $\underline{y}(0)$! System is called *ergodic*.

Example for non-ergodic system:




$\boxed{\text{Target: Choose } W_{\underline{y}\underline{z}} \text{ such that } P_{ST} = P}$

Since $P(.)$ time-independent, from (54) with

$$0 = \Delta P(\underline{y}) = \sum_{\underline{z}} W_{\underline{z}\underline{y}} P(\underline{z}) - \sum_{\underline{z}} W_{\underline{y}\underline{z}} P(\underline{y}) \quad \forall \underline{y}$$

one has more conditions for transition probabilities.

Can be fulfilled, e.g. by

$$W_{\underline{z}\underline{y}} P(\underline{z}) - W_{\underline{y}\underline{z}} P(\underline{y}) = 0 \quad \forall \underline{y}, \underline{z} \tag{55}$$

(called *detailled balance*).

Thus: Markov process generates state distributed according to $P(.)$.
Hence averages (53) can be obtained.

Attention: at beginning states depend on $\underline{y}(0)$
$\Rightarrow$ states for $t < t_{equi}$ or omitted from average calculation ("equilibration").

$\underline{y}(t+1)$ typically "similar" to $\underline{y}(t)$
$\Rightarrow$ only distant states $\underline{y}(t), \underline{y}(t+\Delta t), \underline{y}(t+2\Delta t), \ldots$ are almost independent.

Remark: $t_{equi}, \Delta t$ depend STRONGLY on model, algorithm and parameters
$\Rightarrow$ have to be determined experimentally in simulations.

VIDEO: `video08c_metropolis_r`

## 11.2 Disordered (diluted) Ferromagnet

Model:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} e_i s_i e_j s_j \quad J > 0. \tag{56}$$

$\langle i, j \rangle$ : sum over interacting neighbors (e.g. next neighbours)
$e_i = 0, 1$ : site free/occupied
$s_i = \pm 1$ : spin orientation "up"/ "down".
configuration: $\underline{x} = (s_1, s_2 \ldots, s_N)$ (spins with $e_i = 0$ are effectivly ignored)

Target: simulation in *canonical ensemble*:

$$P(\underline{x}) = \frac{1}{Z} \exp(-\mathcal{H}(\underline{x})/T)\,, \tag{57}$$

with $Z =$ partition function $Z = \sum_{\{\underline{x}\}} \exp(-\mathcal{H}(\underline{x})/T)$.

Method: use Markov chain.

Here:
Metropolis Algorithmus defined by transition probabilities $W_{\underline{y}\underline{z}} = W(\underline{y} \to \underline{z})$.

Basic idea: (given $\underline{y} = \underline{y}(t)$)

1. Create *test configuration* $\underline{z}$ *randomly*, according to $A(\underline{y} \to \underline{z})$

2. With probability $\tilde{W}(\underline{y} \to \underline{z})$ $\underline{z}$ is *accepted*, i.e. $\underline{y}(t+1) = \underline{z}$.
   $\tilde{W}(\underline{y} \to \underline{z})$ is called *acceptance probability*

   With probability $1 - \tilde{W}(\underline{y} \to \underline{z})$ $\underline{z}$ is *rejected*, i.e. $\underline{y}(t+1) = \underline{y}$

$\to$ Full probability:

$$W(\underline{y} \to \underline{z}) = A(\underline{y} \to \underline{z}) \tilde{W}(\underline{y} \to \underline{z}) \quad (\underline{y} \neq \underline{z})\,. \tag{58}$$

(probability that state $\underline{y}$ remains: $W(\underline{y} \to \underline{y}) = 1 - \sum_{\underline{z} \neq \underline{y}} W(\underline{y} \to \underline{z})$).

Insert Eq. (58) into detailled balance condition

$$\frac{\tilde{W}(\underline{y} \to \underline{z})}{\tilde{W}(\underline{z} \to \underline{y})} = \frac{P(\underline{z})}{P(\underline{y})} \frac{A(\underline{z} \to \underline{y})}{A(\underline{y} \to \underline{z})}\,. \tag{59}$$

For Metropolis algorithmus [8], choice:

$$\tilde{W}(\underline{y} \to \underline{z}) = \min\left(1, \frac{P(\underline{z})}{P(\underline{y})}\frac{A(\underline{z} \to \underline{y})}{A(\underline{y} \to \underline{z})}\right), \tag{60}$$

One sees easily that Eq. (59) holds.

Most simple: single-spin flip dynamics:
Let $\underline{y} = (s_1, s_2, \ldots, s_N)$. Choose a spin $j$ randomly, then $\underline{z} = (s'_1, s'_2, \ldots, s'_N)$ with

$$s'_i = \begin{cases} -s_i & \text{for } i = j \\ s_i & \text{else} \end{cases}$$

All spins equal likely: $A(\underline{y} \to \underline{z}) = 1/N$
(better: choose among spins $e_i \neq 0$: $A(\underline{y} \to \underline{z}) = 1/(\sum_i e_i)$)

[Activator]

What is the result for the Boltzmann distribution when inserting into (Metropolis Acceptance probability) ?

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Acceptance probability depends only on *energy change* $\Delta\mathcal{H} = \mathcal{H}(\underline{z}) - \mathcal{H}(\underline{y})$
$\Rightarrow$ easy to compute, because only neighbors $N(j)$ of $j$ contribute:
$\Delta\mathcal{H} = \Delta\mathcal{H}(j) = 2J\sum_{i\in N(j)} e_i s_i e_j s_j$
Obervation: at low temperatures, changes which increase energy are rarely accepted.
Since at most on spin flipped: algorithm is slow, configurations change globaly only on large time scales.
Slowest: Close to phase transitions. (Solution here: cluster algorithms).
Summary:

**algorithm** MC Ferromagnet
**begin**
    **for**(MC iterations)
    **begin**
        select occupied site $t$ randomly
        $\Delta H = 0$
        **for**(all neighbors of $t$ )
            add contribution to $\Delta H$
        flip spin with Metropolis probability($\Delta H$)
    **end**
**end**

VIDEO: `video08d_messgroessen_r.mkv`

## 11.3 Ferromagnet: oservables

Repetition:
Average magnetisation:

$$\langle m\rangle = \frac{1}{Z}\sum_{\{\underline{s}\}} m(\underline{s})\exp(-\beta H(\underline{s})) \tag{61}$$

with $m=\sum_i s_i/N$, $Z=\sum_{\{\underline{s}\}}\exp(-\beta H(\underline{S}))$, $\beta=1/k_BT$, $N=L^d$ spins.
Small magnetic field $B$: $H_B(\underline{s}) = -\sum_{\langle i,j\rangle} s_i s_j - B\sum_i s_i \to$

[Activator]

Calculate $\frac{\partial Z}{\partial B}\Big|_{B=0}$

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For the suszeptibility

$$\begin{aligned}
\chi &\equiv \frac{\partial\langle m\rangle}{\partial B}\Big|_{B=0} \\
&= \frac{\partial}{\partial B}\Big|_{B=0}\frac{1}{Z}\sum_{\{\underline{s}\}} m\exp(-\beta H(\underline{s})) \\
&= -\frac{1}{Z^2}\frac{\partial Z}{\partial B}\Big|_{B=0}\sum_{\{\underline{s}\}} m\exp(-\beta H(\underline{s})) + \frac{1}{Z}\frac{\partial}{B}\Big|_{B=0}\sum_{\{\underline{s}\}} m\exp(-\beta H(\underline{s})) \\
&= -\frac{1}{Z^2}\beta N\left(\sum_{\{\underline{s}\}} m\exp(-\beta H(\underline{s}))\right)^2 + \frac{1}{Z}\beta N\sum_{\{\underline{s}\}} m^2\exp(-\beta H(\underline{s})) \\
&= \beta N\left(\langle m^2\rangle - \langle m\rangle^2\right) = \beta N\sigma^2
\end{aligned} \tag{62}$$

Determination of phase transition: *Binder cumulant* of magnetization

$$b(L,T) = 0.5\left(3-\frac{\langle m^4\rangle}{\langle m^2\rangle^2}\right) \tag{63}$$

One can show:

- $b(L,T)$ curves for different $L$ intersect (almost) at $T_c$.
- Average absolute magnetisation per spin $M \equiv \langle |m| \rangle$ behaves (theory of phase transitions):

$$M(T) \sim |T - T_c|^\beta \quad (T < T_c) \tag{64}$$

  For finite systems

$$M(T, L) = L^{-\beta/\nu} \tilde{\xi}_1(L/\xi) = L^{-\beta/\nu} \hat{\xi}_1(L^{1/\nu}(T - T_c))$$

  where $\nu$ describes the divergence of the correlation length at the critical point.