Course 10/2

Correlated sampling

- Motivation
- Markovian chain
- Theorem associated to a Markovian chain
- Scope in correlated sampling

Motivation

$$I = \frac{\iiint dx_1 dx_2 \ldots dx_d \; f(x_1, x_2, .., x_d) \exp[-\beta E(x_1, x_2, .., x_d)]}{\iiint dx_1 dx_2 \ldots dx_d \; \exp[-\beta E(x_1, x_2, .., x_d)]} \qquad \beta = \frac{1}{kT}$$

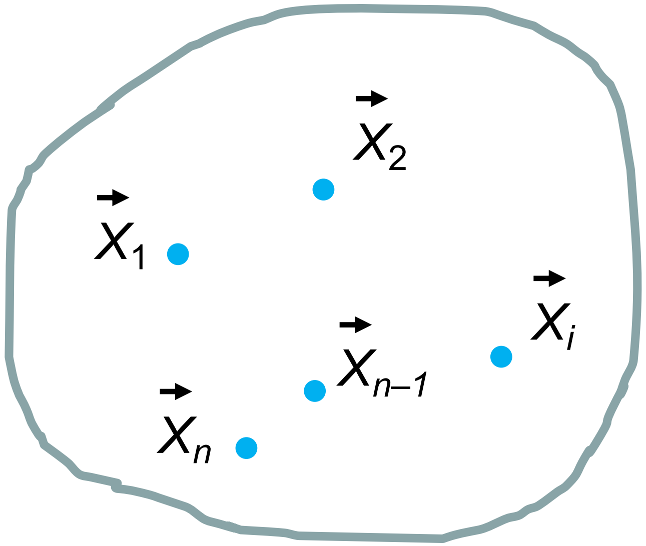
weight function $\omega(x_1, x_2, \ldots. x_d)$

We need a method for generating random variables according to a given weight function $\omega(x_1, x_2, \ldots. x_d)$.

Von Neuman's method will be impractical because the exponential dependence of the weight function will result in many rejections.

Uncorrelated sampling

So far, we chose configurations $\vec{X}_i$ in phase space in a random sequence in which the selection of each successive configuration was independent from the previous one.

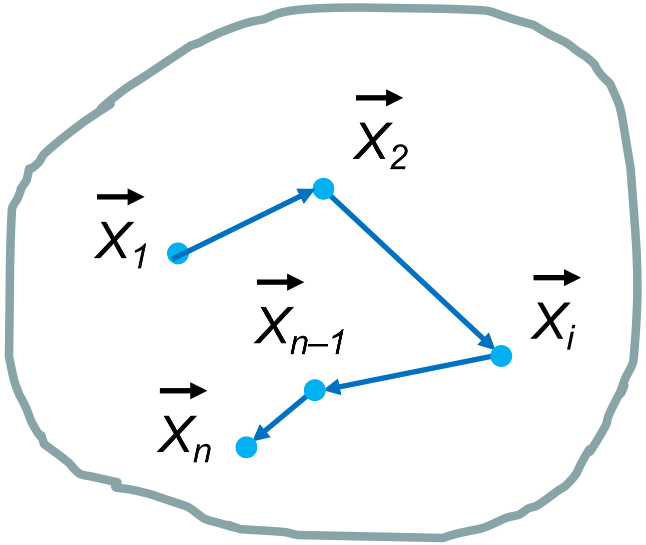


The probability of such a sequence is given by:

$$P_n(\vec{X}_1, \vec{X}_2, \ldots \vec{X}_n) = P(\vec{X}_1) \cdot P(\vec{X}_2) \cdot \cdot \cdot \cdot P(\vec{X}_n)$$

We now abandon the idea of statistical independence.
For calculating integrals, this is not necessary.
What is important is the correct description of the weight function.

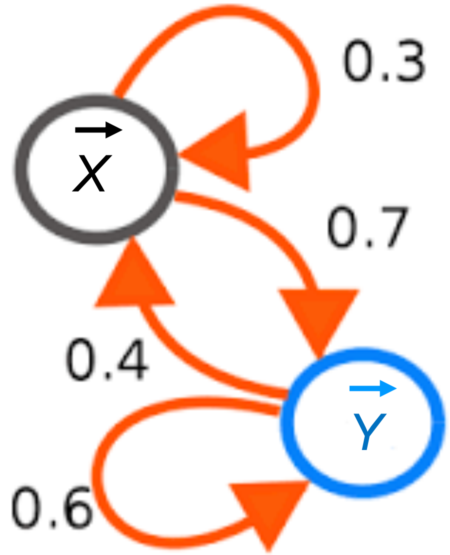
Markovian chain



We introduce the concept of Markovian chain. The probability for such a sequence can be written as:

$$P_n(\vec{X}_1, \vec{X}_2, \ldots \vec{X}_n) = P(\vec{X}_1) \cdot P(\vec{X}_1 \to \vec{X}_2) \cdot P(\vec{X}_2 \to \vec{X}_3) \cdot \cdot \cdot \cdot P(\vec{X}_{n-1} \to \vec{X}_n)$$

where $P(\vec{X} \to \vec{X}')$ only depends on the two points in phase space, not on the history of the chain.

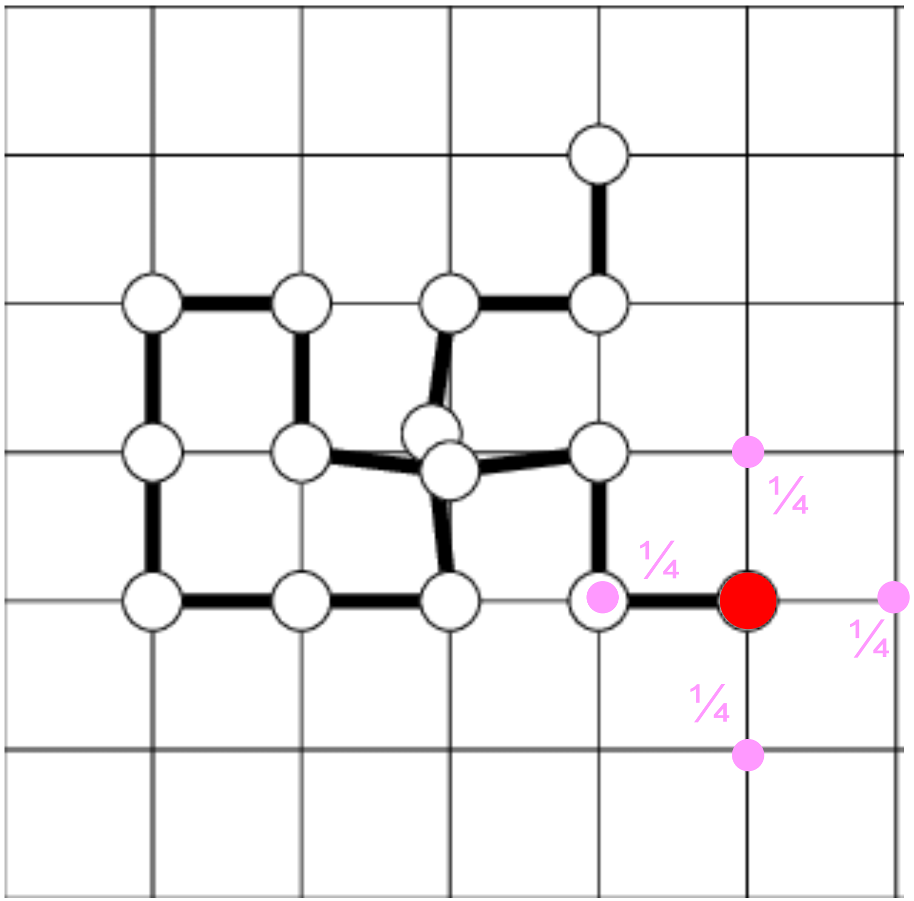


The transition probabilities additionally satisfy the condition:

$$\sum_{\vec{X}'} P(\vec{X} \to \vec{X}') = 1$$

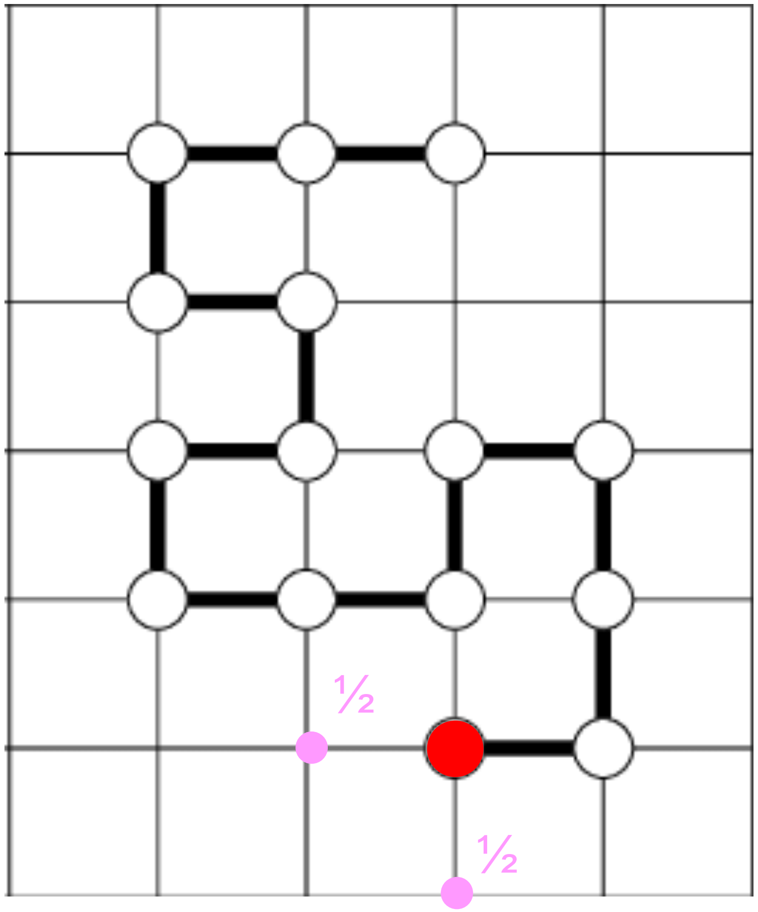
Examples

Random walk in 2D



This is a Markovian chain

Self-avoiding random walk in 2D



This is NOT a Markovian chain

Theorem associated to a Markovian chain

Under the condition of ergodicity, a Markovian chain yields an invariant (stationary) distribution $\rho(\vec{X})$ for the probability of occupation of the configuration sites $\vec{X}$, at least for long times after the start.

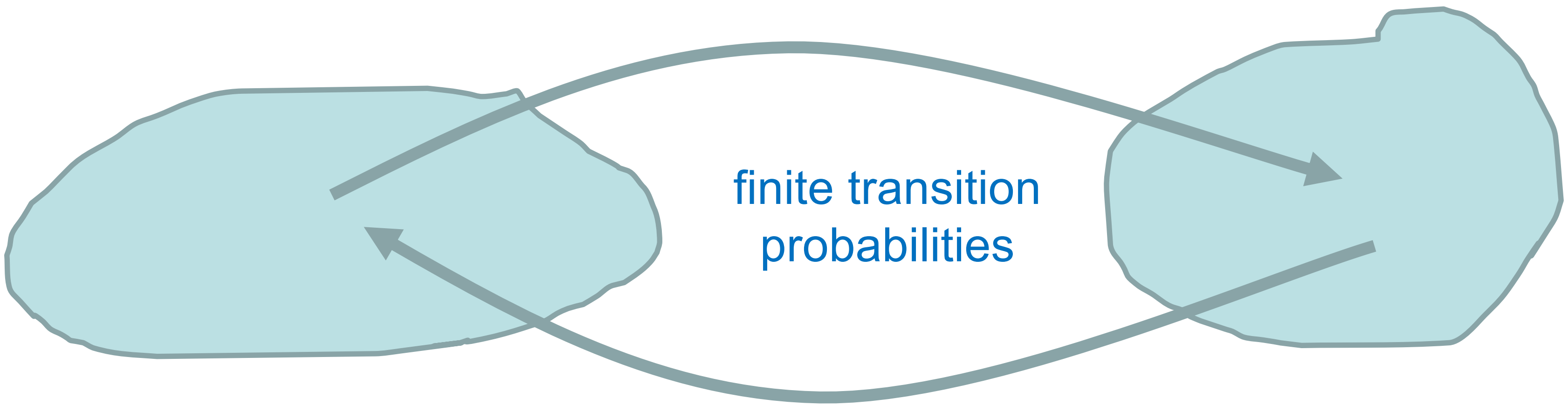
Markovian chain
i.e. definition of all
transition probabilities
$P(\vec{X} \rightarrow \vec{X}')$

$\Rightarrow$

Invariant distribution
$\rho(\vec{X})$

Conditions of ergodicity

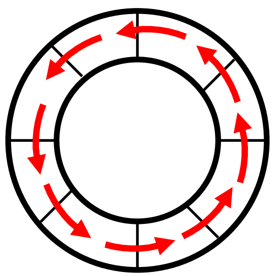
1. Every configuration is accessible from every other one within a finite number of steps ≡ phase space is “connected”.



2. There is no periodicity.

   Periodicity ≡ one can return to a given configuration only by multiples of *k* steps.

   Example of periodicity:



Notion of walkers

The theorem applies to the average occupation of each configuration as the chain proceeds.

Similarly, if one allows several independent Markovian chains to evolve simultaneously, then the theorem applies to the instantaneous distribution of the heads of the chains. These are called walkers.

The population of walkers in a generic configuration $\vec{X}$ becomes stationary and proportional to $\rho(\vec{X})$.

Scope in correlated sampling

Define $P(\vec{X} \to \vec{X}')$ in such a way that the invariant distribution targets the desired weight function:

$$\boxed{\rho(\vec{X}) = \omega(\vec{X})}$$

Then

$$I = \iiint f(x_1, x_2, .., x_d)\ \omega(x_1, x_2, \ldots, x_d)\, dx_1 dx_2 \ldots dx_d \cong \frac{1}{N} \sum_{n=1}^{N} f(x_1^n, x_2^n, \ldots, x_d^n)$$

provided the Markovian chain has reached equilibrium

There is some freedom …

setting

$P(\vec{X} \rightarrow \vec{X}')$

$\Rightarrow$

$\omega(\vec{X}) = \rho(\vec{X})$

Suppose we have a finite number of configurations N.

$N \times N$

$\Rightarrow$

N

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