Stochastic Simulation
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We recall some concepts on the theory of Markov chains on a discrete state space X.

Irreducibility

Let P be be a transition matrix on X. We say that a state $x_i \in X$ communicates with a state $x_j \in X$ if $\mathbb{P}(X_n = x_j,\ \text{for some } n \mid X_0 = x_i) > 0$; equivalently, if $\exists n \geqslant 0$ such that $P_{i,j}^{(n)} > 0$. A Markov chain is *irreducible* if every state x_j communicates with every other state x_i, i.e.,

$$\forall i, j, \quad \exists n \geqslant 0 \text{ such that } P_{i,j}^{(n)} > 0.$$

Recurrence

A state $x_i \in X$ is *recurrent* if $\mathbb{P}(X_n = x_i \text{ infinitely often }) = 1$, that is, x_i is visited infinitely-often with probability 1. A Markov chain $\{X_n\}$ is recurrent if every state is recurrent. It is known that every irreducible recurrent Markov chain $\{X_n\}$ on a discrete state space has a (not necessarily finite) invariant distribution π that is unique up to a multiplicative constant. However, if the state space is *finite*, every irreducible Markov chain $\{X_n\}$ is recurrent and has a unique invariant probability distribution.

Aperiodicity

The *period* of a state x_i is the largest integer d satisfying the following property: $P_{i,i}^{(n)} = 0$, whenever n is not divisible by d. The period of x_i is given by $d(i)$. We say that if $d(i) > 1$, then the state x_i is *periodic*. We say that the state x_i is *aperiodic* otherwise. If a Markov chain $\{X_n\}$ is irreducible and has an aperiodic state, then all states are aperiodic, in which case we say that $\{X_n\}$ is aperiodic. In particular, an irreducible Markov chain $\{X_n\}$ is aperiodic if there exists a state $x_j \in X$ such that $P_{jj} > 0$. It is known that an irreducible Markov chain $\{X_n\}$ on a *finite* state space X converges to π, i.e., $\pi_j = \lim_{n\to\infty} \mathbb{P}(X_n = x_j)$, $x_j \in X$, if and only if $\{X_n\}$ is aperiodic.

Exercice 1.

A random walk on the integers $I = \{0, 1, 2 \dots\}$ can be constructed in the following way. For $0 < p < 1/2$, let $Y_0, Y_1, \dots$ be i.i.d random variables with $P(Y_i = 1) = p$ and $P(Y_i = -1) = 1 - p$. Define two random walks as (1) $X_n = \max\{X_{n-1} + Y_n, 0\}$ and (2) $Z_n = |Z_{n-1} + Y_n|$.

1) Show that (X_n) and (Z_n) are Markov chains.

2) Show that an invariant measure of the chains (X_n) and (Z_n) is given by

$$\hat{\pi} = \left[1, \left(\frac{p}{1-p}\right), \dots, \left(\frac{p}{1-p}\right)^k, \dots\right] a_0, \quad k \geqslant 0$$
$$\bar{\pi} = \left[1, \frac{1}{1-p}, \frac{p}{(1-p)^2}, \dots, \frac{p^{k-1}}{(1-p)^k}, \dots\right] b_0, \quad k \geqslant 1,$$

respectively. Find a_0, b_0 such that the expressions above are probability distributions.

3) Let $p = 1/8$. Assess numerically the convergence of both Markov chains to their invariant distribution by simulating multiple (independent) chains of length $n = 100$, each starting in 0 (i.e. $\lambda = \delta_0$). That is, plot the empirical distribution of X_n, Z_n vs $\hat{\pi}$ and $\bar{\pi}$, respectively. Repeat your experiments for $m = n + 1$. Explain your results.

4) Discuss the periodicity of both chains.

Exercice 2.

Given the transition matrix

$$P = \begin{pmatrix} 0.0 & 0.4 & 0.6 & 0.0 & 0.0 \\ 0.65 & 0.0 & 0.35 & 0.0 & 0.0 \\ 0.32 & 0.68 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.12 & 0.88 \\ 0.0 & 0.0 & 0.0 & 0.56 & 0.44 \end{pmatrix}, \qquad (2.1)$$

and examine whether the corresponding chain is irreducible and aperiodic.

Exercice 3.

Let us consider a 2D uniform square-lattice with atoms placed at each vertex, as is sketched in Figure 1. The atoms can have an upward (red arrow) or a downward (blue arrow) pointing magnetic moment (so-called *spin*). Specifically, let the lattice be made out of $m \times m$ atoms. Therefore the system's possible states are the 2^{m^2} possible spin choices for the m^2 atoms. That is, the spin of the atom at position (i, j) in the lattice is denoted with s_{ij}, $1 \leqslant i, j \leqslant m$, and can take a value in $\{-1, +1\}$. A specific system configuration is described by the matrix $S = (s_{ij}) \in \{-1, +1\}^{m \times m}$, containing the spin of each of the m^2 atoms.

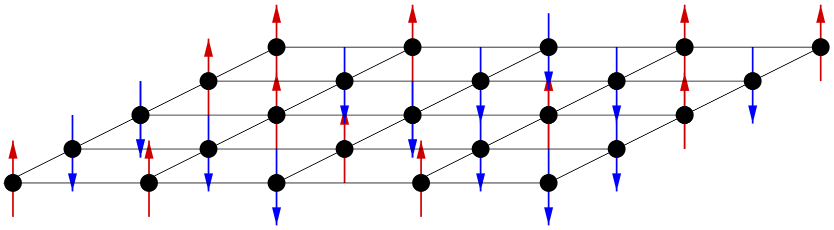

Figure 1: Sketch of 2D square-lattice Ising model.

The energy of a given system state of this Ising model is given by

$$H(S) = -\sum_{i,j=1}^{m} \left(\frac{1}{2} J s_{ij}(s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1}) + B s_{ij} \right) , \tag{3.1}$$

where J is a magnetic coupling constant and B is a constant describing the external magnetic field. To account for boundary effects, we set $s_{0,j} = s_{j,0} = s_{m+1,j} = s_{j,m+1} = 0$ in (3.1). The probability of obtaining a specific system state is then given by the *Boltzmann* distribution with Probability Mass Function (PMF)

$$f(S) \equiv f_\beta(S) = \frac{1}{Z_\beta} e^{-H(S)\beta} , \tag{3.2}$$

where $\beta = 1/(k_B T)$ denotes the so-called inverse-temperature (or thermodynamic beta) with k_B being the Boltzmann constant and T the absolute temperature. Here, Z_β denotes the normalization constant that makes the target distribution $f_\beta \colon \{-1, +1\}^{m\times m} \to \mathbb{R}_+$ a proper PMF.

Let's denote by $M(S) = \sum_{i,j=1}^{m} s_{ij}/m^2$ the system's average magnetic moment corresponding to the configuration S. Notice that the random realizations of the configuration matrix S depend on the inverse temperature β. The expected value of the average magnetic moment $\overline{M}(\beta)$ as a function of the inverse temperature β thus reads

$$\overline{M}(\beta) = \sum_{S\in\mathcal{K}} M(S) f_\beta(S) = \frac{1}{Z_\beta} \sum_{S\in\mathcal{K}} M(S) e^{-H(S)\beta} , \tag{3.3}$$

where $\mathcal{K} = \{-1, 1\}^{m\times m}$ is the set of all possible system configurations. Since the explicit computation of the normalization constant Z_β is computationally expensive (Explain why!), we rely on the Metropolis–Hastings algorithm here. That is, at each step a candidate configuration is proposed by randomly choosing an atom, with uniform probability, and "flipping" its spin.

1) Write a `Python` function that implements the Metropolis–Hastings algorithm for the Ising model. The input parameters for your function are: the number of steps n of the chain that should be simulated, the number of atoms m^2, the inverse temperature β, the constants J and B, and the initial state of the system. The function should return a list of energies and mean magnetic moments computed for each step of the chain, as well as the final configuration of the system.

2) Use your `Python` function with $\beta = 1/3$ and for n, such that both the energy and the average magnetic moment appear to have reached stationarity. Plot also the final system configuration. Furthermore, compute the mean magnetic moment $\overline{M}(\beta)$ for different values of $\beta \in [\frac{1}{3}, 1]$ and $n = 5 \cdot 10^6$. Choose a lattice of 50×50 atoms, $J = 1$, and $B > 0$ for all simulations.

3) Show that the Markov Chain obtained via the Metropolis-Hastings algorithm in this case is irreducible.

Exercice 4.

Consider a Random Walk $(X_n)_n$ on the integers $\mathbb{Z} = \{0, \pm 1, \pm 2, \dots\}$ with transition probabilities given by

$$\mathbb{P}(X_{n+1} = i+1 | X_n = i) = p, \quad \mathbb{P}(X_{n+1} = i-1 | X_n = i) = q = 1-p,$$

where $0 < p < 1$. Address the following points.

1) Show that the chain is irreducible.

2) Conclude for each value of p if the chain is recurrent or transient by computing $\mathbb{E}(V_0)$, where V_0 denotes the number of visits of the state 0. (*Hint*: use Stirling's approximation $n! \sim (n/e)^n\sqrt{2\pi n}$.)

Now consider a symmetric Random Walk on $\mathbb{Z}^2$ with

$$\mathbb{P}(X_{n+1} = (i \pm 1, j)|X_n = (i, j)) = \mathbb{P}(X_{n+1} = (i, j \pm 1)|X_n = (i, j)) = \frac{1}{4}.$$

Address the following points.

3) Show that the chain is irreducible.

4) Conclude that the chain is recurrent by computing $\mathbb{E}(V_0)$, where V_0 denotes the number of visits of the state $(0, 0)$. (*Hint*: use the identity $\binom{2n}{n} = \sum_{i=0}^{n} \binom{n}{i}\binom{n}{n-i}$ and Stirling's approximation.)