

## Lecture 4: Markov chains

**Exercise** Draw the digraphs and classify the states of the Markov chains defined by the following transition matrices:

$$(A) \quad \mathcal{P} = \begin{pmatrix} 0 & 0 & 0.5 & 0.5 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (B) \quad \mathcal{P} = \begin{pmatrix} 0.3 & 0.4 & 0 & 0 & 0.3 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.6 & 0.4 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (4)$$

**Exercise** Consider the Markov chain with transition matrix

$$\mathcal{P} = \begin{pmatrix} 1/2 & 1/3 & 1/6 \\ 3/4 & 0 & 1/4 \\ 0 & 1 & 0 \end{pmatrix} \quad (5)$$

- (a) Show that the MC is irreducible and aperiodic
- (b) Suppose to start the process in state 1; find the probability that it is in state 3 after two steps.
- (c) Find the matrix which is the limit of  $\mathcal{P}^n$  as  $n \rightarrow \infty$ .

**Exercise** Two boxes, A and B, contain 2 white and 3 red balls respectively. At each time one extracts one ball from each box, and puts it back in the opposite box (1 event). Let us call by  $a_1$  the state corresponding to the number  $i$  of the red balls in box A. Determine the occurrence probability of state  $a_2$  after 3 events and in the limit of many events.

## Lecture 5: MC simulation of a 2D Ising model by the Metropolis algorithm

**Program** Write a program that simulates a 2D Ising model with periodic boundary conditions by using the Metropolis acceptance matrix  $a_{ij}$  and the matrix  $\Gamma_{ij}$  based on the local spin-flip (Glauber) proposed move.

**Simulation** By assuming  $k_B = 1$  and  $J = 1$  simulate the 2D Ising model for different values of temperatures (at least 3, one below, one above, and one close to the critical temperature  $T_c = \frac{2}{\ln(1+\sqrt{2})}$  and 3 different values of  $L$  (for instance 25, 50 and 100).

**Equilibration time, averages and fluctuations** After having determined the equilibrium time and disregarding the samples for  $t < \tau_{eq}$  estimate the ensemble averages of the magnetisation per spin, the energy per spin, and the corresponding fluctuations (specific heat and magnetic susceptibility).

**Integrated correlation time and critical slowing-down** Estimate the autocorrelation time of the magnetisation and the energy for the MC simulations proposed above and estimate the errors accordingly.