Math 450 - Homework 6
Solutions

1. Exercise 1.7.1. Find all the invariant distributions of the transition matrix

$$P = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

We need to solve the system $\pi = \pi P$ with the extra normalization condition $\sum_i \pi_i = 1$. These give the 6 equations"

$$\begin{aligned} \pi_1 &= \frac{1}{2}\pi_1 + \frac{1}{2}\pi_5 \\ \pi_2 &= \frac{1}{2}\pi_2 + \frac{1}{4}\pi_4 \\ \pi_3 &= \pi_3 + \frac{1}{4}\pi_4 \\ \pi_4 &= \frac{1}{2}\pi_2 + \frac{1}{4}\pi_4 \\ \pi_5 &= \frac{1}{2}\pi_1 + \frac{1}{4}\pi_4 + \frac{1}{2}\pi_5 \\ 1 &= \pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5. \end{aligned}$$

There are 4 independent homogeneous equations and the non-homogeneous normalizing condition. Eliminating the second to last equation and writing the system in standard matrix form gives:

$$\begin{pmatrix} -\frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} & 0 \\ 0 & \frac{1}{2} & 0 & -\frac{3}{4} & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \pi_1 \\ \pi_2 \\ \pi_3 \\ \pi_4 \\ \pi_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

This gives $\pi_1 = \pi_5$, $\pi_2 = \pi_4 = 0$, and $\pi_1 + \pi_3 + \pi_5 = 1$. Thus invariant measures must have the form $\pi = (a, 0, b, 0, a)$ where a, b are non-negative and $2a + b = 1$, and any such distribution is an invariant probability measure. Note that the transient states 2 and 4 must have probability 0.

2. Exercise 1.7.2. (Ehrenfest model) Gas molecules move about randomly in a box which is divided into two halves symmetrically by a partition. A hole is made in the partition. Suppose there are N molecules in the box. Think of the partitions as two urns containing balls labeled 1 through N. Molecular motion can be modeled by choosing a number between 1 and N at random and moving the corresponding ball from the urn it is presently in to the other. This is a historically important physical model introduced by Ehrenfest in the early days of statistical mechanics to study thermodynamic equilibrium.

   (a) Show that the number of molecules on one side of the partition just after a molecule has passed through the hole evolves as a Markov chain. What are the transition probabilities? (Take as the sets of states the number of molecules in one of the partitions.) Draw a transition diagram of the process.
   The set of states of the Markov chain is

$$S = \{0, 1, 2, \ldots, N\}$$

   representing the number of molecules in one partition of the box. The transition probabilities are as follows:

$$P(X_{n+1} = j | X_n = i) = \begin{cases} i/N & \text{if } j = i - 1 \\ (N - i)/N & \text{if } j = i + 1. \end{cases}$$

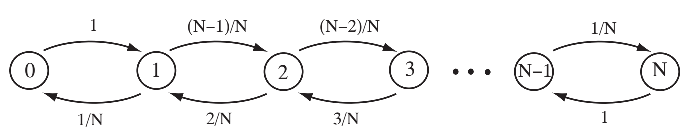

Figure 1: Transition diagram for the Ehrenfest gas model.

   (b) Is the chain recurrent? Yes. This is an irreducible finite chain, so all states are recurrent.

   (c) What is the invariant distribution of this chain? We use the notation $p_i = (N - i)/N$ and $q_i = i/N$. Then $\pi = \pi P$ corresponds to the following system of equations:

$$\begin{aligned} \pi_0 &= \pi_1 q_1 \\ \pi_1 &= \pi_0 p_0 + \pi_2 q_2 \\ \pi_2 &= \pi_1 p_1 + \pi_3 q_3 \\ &\cdots \\ \pi_i &= \pi_{i-1} p_{i-1} + \pi_{i+1} p_{i+1} \\ &\cdots \\ \pi_N &= \pi_{N-1} p_{N-1}. \end{aligned}$$

A simple induction shows that the unique solution (up to a multiplicative constant, which is determined by the equation $\pi_1 + \cdots + \pi_N = 1$) is given by:

$$\pi_i = \frac{p_{i-1}p_{i-2}\cdots p_0}{q_i q_{i-1}\cdots q_1}\pi_0.$$

From this we obtain:

$$\pi_i = \pi_0 \frac{(N-i+1)(N-i+2)\ldots N)}{i(i-1)\ldots 1} = \pi_0 \frac{N!}{i!(N-i)!} = \pi_0 C(N,i).$$

To find π_0, notice that the sum of the binomial coefficients is 2^N, so from $\pi_0 + \cdots + \pi_N = 1$ we get $\pi_0 = 1/2^N$. Therefore,

$$\pi_i = \frac{C(N,i)}{2^N}.$$

(d) What is the number of steps it takes on average for a partition to become empty given that it was initially empty? In other words, find the expected return time to state 0.

We wish to find $m_0 = E_0[T_0]$. According to theorem 1.7.7, and since the chain is recurrent, this is given by

$$m_0 = \frac{1}{\pi_0} = 2^N.$$

If $N = 100$, and assuming each transition takes about 1/400th of a second, the mean return time to an empty partition is $2^{100}/400$ seconds. This is over 10^{18} centuries.

(e) Do a computer simulation of this Markov chain for $N = 100$. Start from state 0 (one of the partitions is empty) and follow the chain up to 1000 steps. Draw a graph of the number of molecules in the initially empty partition as a function of the number of steps. On the basis of your answer to the previous item, would you expect to observe during the course of the simulation a return to state 0?

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
rand('seed',327)
tic
%number of molecules:
N=100;
%number of time steps:
t=1000;
%States are represented by
%row vectors whose ith entry is zero
%if ith molecule is in second
%compartment, and one if it is in the first.
%We start with and empty first compartment:
```

```
s=zeros(1,N);
%Number of molecules in first compartment:
number=[sum(s)];

for j=1:t
    %choose at random a number between 1 and N:
    i=ceil(N*rand);
    %Let 0 represent the first compartment and 1 the
    %second. Moving molecule i to a different
    %compartment means switching ith entry of s
    %from 0 to 1 or vice-versa.
    s(i)=rem(s(i)+1,2);
    number=[number sum(s)];
end
plot(0:t,number)
grid
toc
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

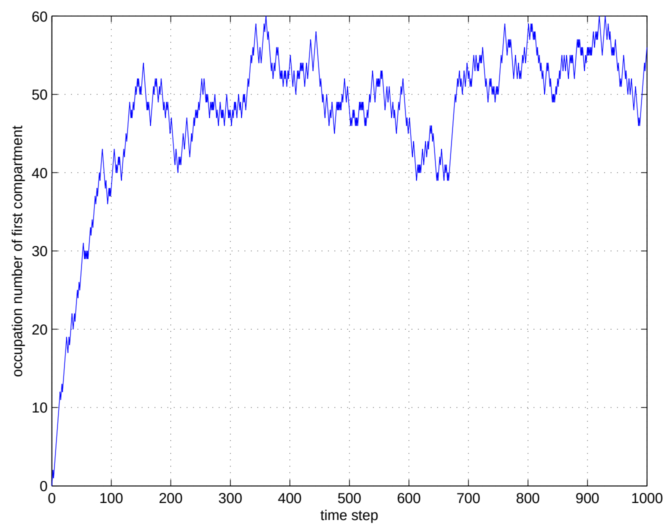

Figure 2: Number of molecules in the first compartment as a function of time. Time is measured in number of steps of the discrete Markov chain.

3. Exercise 1.7.3. A particle moves on the eight vertices of a cube in the following way: at each step the particle is equally likely to move to each of the three adjacent vertices, independently of its past motion. Let i be the

initial vertex occupied by the particle, o the vertex opposite i. Calculate each of the following quantities:

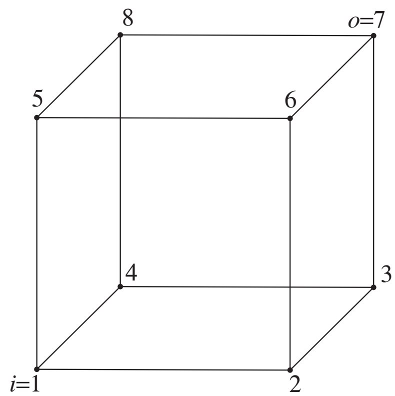

Figure 3: Transition diagram for the random walk on the cube. Each transition has probability 1/3.

(a) The expected return time to i is given by $E_i[T_i] = 1/\pi_i$, where π is the stationary probability distribution vector. This is unique since the chain is irreducible and finite. It is easy to show that the constant distribution $\pi_j = 1/8$ (suggested by symmetry) is stationary. Therefore,

$$E_i[T_i] = 8.$$

(b) The expected number of visits to o until the first return to i is given by theorem 1.7.5 as the number γ_o^i such that the vector $\gamma^i = (\gamma_1^i, \dots, \gamma_8^i)$ satisfies: $\gamma_i^i = 1$, $0 < \gamma_j^i < \infty$, and $\gamma^i P = \gamma^i$. By theorem 1.7.6, this is a constant vector, $\gamma_j^i = 1$ for all j. Therefore,

$$\gamma_o^i = 1.$$

(c) The expected number of steps until the first visit to o can be obtained using theorem 1.3.5. We write k_j^o for the number of steps until first visit to o, starting at j. We simplify the system using symmetry considerations. Write $u = k_2^o = k_4^o = k_5^o$, $v = k_3^o = k_6^o = k_8^o$, $k = k_1^o$, and $k_7^o = 0$. (We want the value of k.) The system of theorem 1.3.5 now reduces to the following 3 equations:

$$\begin{aligned} k &= 1 + u \\ u &= 1 + \frac{1}{3}k + \frac{2}{3}v \\ v &= 1 + \frac{2}{3}u. \end{aligned}$$

This is easily solved. The value we want is $k = 10$. ($u = 9$ and $v = 7$.)

To find these values by simulation, we use the following program. It produces sample paths of a Markov chain with initial distribution p and transition probabilities matrix P, stopped at the r-th visit to a set A.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function X=visit(p, P, A, r, n)
%Inputs - p probability distribution of initial state
%       - P transition probability matrix
%       - A set of states where chain is stopped
%       - r number of returns
%       - n maximal time. (If A empty, stop at time n.)
%Output - X sample chain till min{r-th hit time to A, n}.
%
%Note: need function samplefromp.m
q=p;
i=samplefromp(q,1);
X=[i];
m=0;
c=0;
while c<r & m<n-1
    q=P(i,:);
    i=samplefromp(q,1);
    X=[X i];
    c=c+(length(find(A==i))~=0);
    m=m+1;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

We now calculate the mean return time, m_T, to $i = 1$, and the mean number m_N of visits to $o = 7$ between visits to i.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
P=zeros(8,8);
P(1,[2 4 5])=1;
P(2,[1 3 6])=1;
P(3,[2 4 7])=1;
P(4,[1 3 8])=1;
P(5,[1 6 8])=1;
P(6,[2 5 7])=1;
P(7,[3 6 8])=1;
P(8,[4 5 7])=1;
P=(1/3)*P;
p=zeros(1,8);
p(1)=1;
```

```
A=[1];
t=1000;
rand('seed',371)
T=[]; %return time to i=1
N=[]; %number of visites to o=7
for i=1:t
    X=visit(p, P, A, 1, 100000);
    T=[T length(X)-1];
    N=[N sum(X==7)];
end
m_T=mean(T)
m_N=mean(N)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

The above gave the value $m_T = 8.2820$ and $m_N = 1.0650$. (Correct values: 8 and 1, respectively.) For the number of steps till first visit to $o = 7$, starting at $i = 1$, the commands below produce the mean value $m_K = 9.8920$. (Correct value: 10.)

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
A=[7];
t=1000;
rand('seed',371)
K=[]; %number of steps till o=7
for i=1:t
    X=visit(p, P, A, 1, 100000);
    K=[K length(X)-1];
end
m_K=mean(K)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```