Exercises on Markov Chains

Enrico Scalas[1,*]

[1] *Laboratory on Complex Systems. Dipartimento di Scienze e Tecnologie Avanzate, Università del Piemonte Orientale "Amedeo Avogadro", Via Bellini 25 G, 15100 Alessandria, Italy*

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Abstract

These exercises are related to the notes entitled *Summary of results on Markov Chains*.

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*Electronic address: enrico.scalas@mfn.unipmn.it; URL: www.mfn.unipmn.it/~scalas

I. INTRODUCTION

These exercises are based on a very simple agent-based model, the BDY game, described in ref. [1]. The purpose is finding the *stationary* distribution, which in the BDY case is also the *equilibrium* distribution.

At least, there are three different approaches: the direct diagonalization of the transition matrix, Monte Carlo simulation and sampling, and analytical methods. In principle, it is always possible to implement the first two methods, but, for large system sizes these methods may originate untractable numerical problems. The applicability of analytical methods depends on the properties of the investigated model. Below, the case will be discussed in which *detailed balance* holds.

As in many relevant cases, in the BDY case, the state space is finite. For the BDY model, where n objects (coins) must be divided into g categories (agents), the number of states M is given by:

$$M = \binom{n+g-1}{g-1} = \binom{n+g-1}{n}.$$

By construction, the model is a *homogenous* Markov chain and the transition function $P(x, y)$ can be represented by an $M \times M$ matrix. Using the symbols of ref. [1], the transition matrix can be written as:

$$P(\mathbf{n}_i^j|\mathbf{n}) = \frac{1-\delta_{n_i,0}}{g - z_0(\mathbf{n})} \frac{1}{g},$$

where $\mathbf{n}$ is the occupation vector $(n_1, \ldots, n_g)$, n_i is the number of objects in category i and $z_0(\mathbf{n})$ is the number of categories without objects. The meaning of this equation is simply that, in the BDY game, the loser is selected by chance among all the agents having at least one coin and the winner is randomly selected among all the agents (including the loser, so that the coin can come back).

Before studying the stationary and equilibrium distribution, it is necessary to see if there are any *transient* states and/or the states can be divided into separate closed, irreducible sets. If corollary 6 holds true, then the stationary distribution is unique and if the chain is *aperiodic* the stationary distribution is the equilibrium distribution (theorem 13). In the BDY case, the chain is irreducible and aperiodic and there exists a unique equilibrium distribution coinciding with the stationary distribution.

In summary, before studying the stationary distribution it is very useful:

1. to assess the dimension of the state space; this is a not necessarily trivial combinatorial task.

2. to check whether the chain is irreducible (ergodic); this can be done by looking for transient states or by directly verifying whether any state can be reached from any other state.

3. to check whether the chain is aperiodic; also this can be directly done by looking for classes of states with periods with g.c.d. equal to 1.

II. METHOD I: DIAGONALIZATION OF THE TRANSITION MATRIX

As discussed above, this method can be used to study the game when g and n are not too large. To illustrate the method, let us consider the case $g = n = 3$. The total number of occupation states is 10:

$$(0,0,3); (0,3,0); (3,0,0); (1,1,1); (0,1,2); (1,0,2); (1,2,0); (0,2,1); (2,0,1); (2,1,0).$$

The transition matrix between these states can be directly computed by using the rules of the game. For instance, the state $(0,0,3)$ can only go into the three states $(0,1,2)$, $(1,0,2)$ and $(0,0,3)$ with equal probability $1/3$. The state $(0,1,2)$ can go into the five states $(1,0,2)$, $(0,2,1)$, $(1,1,1)$, $(0,0,3)$, and $(0,1,2)$ and each final state can be reached with probability $1/6$ except for state $(0,1,2)$ which can be reached twice over six times and has probability $1/3$. These considerations lead to the following 10×10 transition matrix:

$$\mathbf{P} = \begin{pmatrix} 1/3 & 0 & 0 & 0 & 1/3 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 \\ 0 & 0 & 0 & 1/3 & 1/9 & 1/9 & 1/9 & 1/9 & 1/9 & 1/9 \\ 1/6 & 0 & 0 & 1/6 & 1/3 & 1/6 & 0 & 1/6 & 0 & 0 \\ 1/6 & 0 & 0 & 1/6 & 1/6 & 1/3 & 0 & 0 & 1/6 & 0 \\ 0 & 1/6 & 0 & 1/6 & 0 & 0 & 1/3 & 1/6 & 0 & 1/6 \\ 0 & 1/6 & 0 & 1/6 & 1/6 & 0 & 1/6 & 1/3 & 0 & 0 \\ 0 & 0 & 1/6 & 1/6 & 0 & 1/6 & 0 & 0 & 1/3 & 1/6 \\ 0 & 0 & 1/6 & 1/6 & 0 & 0 & 1/6 & 0 & 1/6 & 1/3 \end{pmatrix}.$$

Either by inspection of the matrix or by building a graph connecting the states, it can be seen that any state leads to any other state, so that this chain is irreducible. Moreover, the period of the chain is one, as there $P(x,x) \neq 0$ for any state x. Therefore this is a finite, irreducible and aperiodic Markov chain. There is a unique stationary ditribution which is also an equilibrium distribution.

The vector, π, giving the equilibrium probability distribution can be computed diagonalizing $\mathbf{P}$, as its transpose, π^t , satisfies: $\pi^t\mathbf{P} = \pi^t$.

In R, one can write the following series of commands:

```
# transition matrix
row1<-c(1/3,0,0,0,1/3,1/3,0,0,0,0)
row2<-c(0,1/3,0,0,0,0,1/3,1/3,0,0)
row3<-c(0,0,1/3,0,0,0,0,0,1/3,1/3)
row4<-c(0,0,0,1/3,1/9,1/9,1/9,1/9,1/9,1/9)
row5<-c(1/6,0,0,1/6,1/3,1/6,0,1/6,0,0)
row6<-c(1/6,0,0,1/6,1/6,1/3,0,0,1/6,0)
row7<-c(0,1/6,0,1/6,0,0,1/3,1/6,0,1/6)
row8<-c(0,1/6,0,1/6,1/6,0,1/6,1/3,0,0)
row9<-c(0,0,1/6,1/6,0,1/6,0,0,1/3,1/6)
row10<-c(0,0,1/6,1/6,0,0,1/6,0,1/6,1/3)
P<-t(matrix(c(row1,row2,row3,row4,row5,row6,row7,row8,row9,row10),nrow=10,ncol=10))
# diagonalization
ev3<-eigen(t(P))
# eigenvalues (the largest eigenvalue is equal to 1)
ev3$val
# eigenvectors (the first column is the eigenvector corresponding to 1)
ev3$vec
# probability of states (the eigenvalue must be normalized)
p<-abs(ev3$vec[,1])/sum(abs(ev3$vec[,1]))
p
# exact values of the equilibrium distribution
pt<-c(1/18,1/18,1/18,1/6,1/9,1/9,1/9,1/9,1/9,1/9)
pt
```

```
# differences
p-pt
p-p%*%P
```

As a final remark one can notice that, as only the eigenvector corresponding to the largest eigenvalue is required, there are efficient numerical methods to compute it.

III. METHOD II: MONTE CARLO SIMULATION

There is not a unique way of implementing a Monte Carlo simulation of the Markov chain described in ref. [1] and outlined above. Below, a simulation is proposed of the 10-state version discussed in the previous section that samples both the transition matrix and the stationary distribution. It is just a tutorial example and more efficient algorithms may be written.

$(1, 1, 1)$ is chosen as the initial state: every category is occupied by one object. Then a couple of categories is randomly selected (first the loser and then the winner) and the loser transfers one object to the winner. If the loser has no objects, nothing happens. Note that the loser can coincide with the winner. It would be possible to be a little bit more efficient, by implementing a periodic version of the program. In this case, the simulation would lead to the same values for the stationary probability distribution, but to a different transition matrix. However, a word of caution is necessary. Sometimes, it is dangerous to use shortcuts of this kind, as one can simulate a different model without immediately realizing it and much time may be necessary to unveil such a bug. For a discussion on this risk, ref. [2] is very useful.

```
# Monte Carlo simulation of the BDY game
# Number of objects
n<-3
# Number of categories
g<-3
# Number of Monte Carlo steps
T<-100000
# Initial occupation vector
y<-c(1,1,1)
```

```
# Frequencies and transitions
state<-4
freq<-c(0,0,0,0,0,0,0,0,0,0)
transmat<-matrix(0,nrow=10,ncol=10)
# Loop of Monte Carlo steps
for (i in 1:T) {
# Random selection of the winner
# Generate a uniformly distributed integer between 1 and 3
indexw<-ceiling(3*runif(1))
# Random selection of the loser
# Generate a uniformly distributed integer between 1 and 3
indexl<-ceiling(3*runif(1))
# Verify if the loser has objects
while(y[indexl]==0) indexl<-ceiling(3*runif(1))
# Dynamic step
y[indexl]<-y[indexl]-1
y[indexw]<-y[indexw]+1
# frequencies
if (max(y)==1) newstate<-4
if (max(y)==3) {
if(y[3]==3) newstate<-1
if(y[2]==3) newstate<-2
if(y[1]==3) newstate<-3
# end if
}
if (max(y)==2) {
if(y[1]==2) { if(y[2]==1) newstate<-10
else newstate<-9
# end if
}
if(y[1]==1) { if(y[2]==2) newstate<-7
else newstate<-6
```

```
# end if
}
if(y[1]==0) { if(y[2]==1) newstate<-5
else newstate<-8
# end if
}
# end if
}
# Updates
freq[newstate]<-freq[newstate]+1
transmat[newstate,state]<-transmat[newstate,state]+1
state<-newstate
# end for
}
# Normalization
freq<-freq/T
freq
for (j in 1:10) transmat[j,]<-transmat[j,]/sum(transmat[j,])
transmat
# Differences
pt<-c(1/18,1/18,1/18,1/6,1/9,1/9,1/9,1/9,1/9,1/9)
pt-freq
row1<-c(1/3,0,0,0,1/3,1/3,0,0,0,0)
row2<-c(0,1/3,0,0,0,0,1/3,1/3,0,0)
row3<-c(0,0,1/3,0,0,0,0,0,1/3,1/3)
row4<-c(0,0,0,1/3,1/9,1/9,1/9,1/9,1/9,1/9)
row5<-c(1/6,0,0,1/6,1/3,1/6,0,1/6,0,0)
row6<-c(1/6,0,0,1/6,1/6,1/3,0,0,1/6,0)
row7<-c(0,1/6,0,1/6,0,0,1/3,1/6,0,1/6)
row8<-c(0,1/6,0,1/6,1/6,0,1/6,1/3,0,0)
row9<-c(0,0,1/6,1/6,0,1/6,0,0,1/3,1/6)
row10<-c(0,0,1/6,1/6,0,0,1/6,0,1/6,1/3)
```

```
P<-t(matrix(c(row1,row2,row3,row4,row5,row6,row7,row8,row9,row10),nrow=10,ncol=10))
P-transmat
```

IV. METHOD III: ANALYTICAL SOLUTION

The analytical solution of the BDY Markov chain rests upon the so-called *detailed balance* property. The solution is discussed in detail in ref. [1]. Here, the focus is on the meaning of detailed balance.

From eq. (9) in the *Summary*, one can derive a *master equation* in the following way (remember that $\sum_x P(y,x) = 1$):

$$P(X_{n+1} = y) - P(X_n = y) = \sum_x P(X_n = x)P(x,y) - P(X_n = y)\sum_x P(y,x)$$

so that

$$P(X_{n+1} = y) - P(X_n = y) = \sum_x [P(X_n = x)P(x,y) - P(X_n = y)P(y,x)].$$

The master equation has an appealing even if somewhat misleading interpretation. The variation in the probability of state y from step n to step $n+1$ is given by a sort of *flow* equation, where the term $P(X_n = x)P(x,y)$ denotes a jump into state y and the term $P(X_n = y)P(y,x)$ denotes a jump leaving state y for another state.

For a stationary distribution $\pi(x)$ one has:

$$\sum_x [\pi(x)P(x,y) - \pi(y)P(y,x)] = 0 \quad (1)$$

A Markov chain is *reversible* with respect to a distribution $\pi(x)$ if for any couple of states x, y, one has

$$\pi(x)P(x,y) = \pi(y)P(y,x). \quad (2)$$

Theorem 1. *If a Markov chain is irreducible, aperiodic and reversible with respect to π, then π is the unique stationary distribution of the chain and is also an equilibrium distribution.*

The proof of this theorem is immediate as π is a stationary distribution:

$$\sum_x \pi(x)P(x,y) = \pi(y)\sum_x P(y,x) = \pi(y)$$

the uniqueness follow from theorem 11, the asymptotic equilibrium property is a consequence of theorem 13. Notice that the reversibility condition is a rather strong one and it imposes a balance of probabilities between any couple of states (hence the name *detailed balance*). In general, for an irreducible chain only the global balance equation (1) holds.

It is worth concluding this discussion with an immediate, but important corollary

Corollary 1. *For a finite irreducible, aperiodic and reversible with respect to* π *Markov chain with symmetric transition function – that is* $P(x, y) = P(y, x)$ *for any couple of states* x *and* y *– the equilibrium probability distribution is uniform.*

This corollary is particularly relevant in statistical physics as it can justify the so-called *postulate of equal a priori probabilities.* A detailed discussion of this point is beyond the scope of these lectures, but the reader is encouraged to read the discussion in ref. [1] showing how *maximum entropy methods* might fail in deriving the correct equilibrium distribution for partitions (the frequency of categories with $0, \ldots, n$ objects).

Acknowledgements

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[1] E. Scalas, U. Garibaldi and S. Donadio, (2006) *Statistical equilibrium in simple exchange games I*, Eur. Phys. J. B, **53**, 267–272. Notice that, in that paper, a $d = 2$ periodic version of this game is considered. For this case, the second part of theorem 13 should apply, but the authors (including myself) failed to add such a remark.

[2] B. Hayes, (2005) *Rumours and Errours*, American Scientist, **93**, 207–211.