# The markovchain Package: A Package for Easily Handling Discrete Markov Chains in R

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#### Abstract

The markovchain package aims to fill a gap within the R framework providing S4 classes and methods for easily handling discrete time Markov chains, homogeneous and simple inhomogeneous ones as well as continuous time Markov chains. The S4 classes for handling and analysing discrete and continuous time Markov chains are presented, as well as functions and method for performing probabilistic and statistical analysis. Finally, some examples in which the package's functions are applied to Economics, Finance and Natural Sciences topics are shown.

Keywords: discrete time Markov chains, continuous time Markov chains, transition matrices, communicating classes, periodicity, first passage time, stationary distributions..

## 1. Introduction

Markov chains represent a class of stochastic processes of great interest for the wide spectrum of practical applications. In particular, discrete time Markov chains (DTMC) permit to model the transition probabilities between discrete states by the aid of matrices. Various R packages deal with models that are based on Markov chains:

- msm (Jackson 2011) handles Multi-State Models for panel data;
- mcmcR (Geyer and Johnson 2013) implements Monte Carlo Markov Chain approach;
- hmm (Himmelmann and www.linhi.com 2010) fits hidden Markov models with covariates:
- mstate fits Multi-State Models based on Markov chains for survival analysis (de Wreede, Fiocco, and Putter 2011).

Nevertheless, the R statistical environment (R Core Team 2013) seems to lack a simple package that coherently defines S4 classes for discrete Markov chains and allows to perform probabilistic analysis, statistical inference and applications. For the sake of completeness, **markovchain** is the second package specifically dedicated to DTMC analysis, being **DTMCPack** (Nicholson 2013) the first one. Notwithstanding, **markovchain** package (Spedicato 2015) aims to offer more flexibility in handling DTMC than other existing solutions, providing S4 classes for both homogeneous and non-homogeneous Markov chains as well as methods suited to perform statistical and probabilistic analysis.

The markovchain package depends on the following R packages: expm (Goulet, Dutang,

Maechler, Firth, Shapira, Stadelmann, and expm-developers@lists.R-forge.R-project.org 2013) to perform efficient matrices powers; **igraph** (Csardi and Nepusz 2006) to perform pretty plotting of markovchain objects and matlab (Roebuck 2011), that contains functions for matrix management and calculations that emulate those within MATLAB environment. Moreover, other scientific softwares provide functions specifically designed to analyze DTMC, as Mathematica 9 (Wolfram Research 2013b).

The paper is structured as follows: Section 2 briefly reviews mathematics and definitions regarding DTMC, Section 3 discusses how to handle and manage Markov chain objects within the package, Section 4 and Section 5 show how to perform probabilistic and statistical modelling, while Section 6 presents some applied examples from various fields analyzed by means of the **markovchain** package. For continuous time Markov chains, refer to the CTMC vignette which is a part of the package.

# 2. Review of core mathematical concepts

### 2.1. General Definitions

A DTMC is a sequence of random variables  $X_1, X_2, \ldots, X_n, \ldots$  characterized by the Markov property (also known as memoryless property, see Equation 1). The Markov property states that the distribution of the forthcoming state  $X_{n+1}$  depends only on the current state  $X_n$  and doesn't depend on the previous ones  $X_{n-1}, X_{n-2}, \ldots, X_1$ .

$$Pr(X_{n+1} = x_{n+1} | X_1 = x_1, X_2 = x_2, ..., X_n = x_n) = Pr(X_{n+1} = x_{n+1} | X_n = x_n).$$
 (1)

The set of possible states  $S = \{s_1, s_2, ..., s_r\}$  of  $X_n$  can be finite or countable and it is named the state space of the chain.

The chain moves from one state to another (this change is named either 'transition' or 'step') and the probability  $p_{ij}$  to move from state  $s_i$  to state  $s_j$  in one step is named transition probability:

$$p_{ij} = Pr(X_1 = s_i | X_0 = s_i). (2)$$

The probability of moving from state i to j in n steps is denoted by  $p_{ij}^{(n)} = Pr(X_n = s_j | X_0 = s_i)$ . A DTMC is called time-homogeneous if the property shown in Equation 3 holds. Time homogeneity implies no change in the underlying transition probabilities as time goes on.

$$Pr(X_{n+1} = s_i | X_n = s_i) = Pr(X_n = s_i | X_{n-1} = s_i).$$
(3)

If the Markov chain is time-homogeneous, then  $p_{ij} = Pr(X_{k+1} = s_j | X_k = s_i)$  and  $p_{ij}^{(n)} = Pr(X_{n+k} = s_j | X_k = s_i)$ , where k > 0.

The probability distribution of transitions from one state to another can be represented into a transition matrix  $P = (p_{ij})_{i,j}$ , where each element of position (i,j) represents the transition

probability  $p_{ij}$ . E.g., if r=3 the transition matrix P is shown in Equation 4

$$P = \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{bmatrix}. \tag{4}$$

The distribution over the states can be written in the form of a stochastic row vector x (the term stochastic means that  $\sum_i x_i = 1, x_i \ge 0$ ): e.g., if the current state of x is  $s_2, x = (0 \ 1 \ 0)$ . As a consequence, the relation between  $x^{(1)}$  and  $x^{(0)}$  is  $x^{(1)} = x^{(0)}P$  and, recursively, we get  $x^{(2)} = x^{(0)}P^2$  and  $x^{(n)} = x^{(0)}P^n$ , n > 0.

DTMC are explained in most theory books on stochastic processes, see Brémaud (1999) and Ching and Ng (2006) for example. Valuable references online available are: ?, Snell (1999) and Bard (2000).

### 2.2. Properties and classification of states

A state  $s_j$  is said accessible from state  $s_i$  (written  $s_i \to s_j$ ) if a system started in state  $s_i$  has a positive probability to reach the state  $s_j$  at a certain point, i.e.,  $\exists n > 0 : p_{ij}^n > 0$ . If both  $s_i \to s_j$  and  $s_j \to s_i$ , then  $s_i$  and  $s_j$  are said to communicate.

A communicating class is defined to be a set of states that communicate. A DTMC can be composed by one or more communicating classes. If the DTMC is composed by only one communicating class (i.e., if all states in the chain communicate), then it is said irreducible. A communicating class is said to be closed if no states outside of the class can be reached from any state inside it.

If  $p_{ii} = 1$ ,  $s_i$  is defined as absorbing state: an absorbing state corresponds to a closed communicating class composed by one state only.

The canonic form of a DTMC transition matrix is a matrix having a block form, where the closed communicating classes are shown at the beginning of the diagonal matrix.

A state  $s_i$  has period  $k_i$  if any return to state  $s_i$  must occur in multiplies of  $k_i$  steps, that is  $k_i = \gcd\{n : \Pr(X_n = s_i | X_0 = s_i) > 0\}$ , where  $\gcd$  is the greatest common divisor. If  $k_i = 1$  the state  $s_i$  is said to be aperiodic, else if  $k_i > 1$  the state  $s_i$  is periodic with period  $k_i$ . Loosely speaking,  $s_i$  is periodic if it can only return to itself after a fixed number of transitions  $k_i > 1$  (or multiple of  $k_i$ ), else it is aperiodic.

If states  $s_i$  and  $s_j$  belong to the same communicating class, then they have the same period  $k_i$ . As a consequence, each of the states of an irreducible DTMC share the same periodicity. This periodicity is also considered the DTMC periodicity.

It is possible to analyze the timing to reach a certain state. The first passage time from state  $s_i$  to state  $s_j$  is the number  $T_{ij}$  of steps taken by the chain until it arrives for the first time to state  $s_j$ , given that  $X_0 = s_i$ . The probability distribution of  $T_{ij}$  is defined by Equation 5

$$h_{ij}^{(n)} = Pr(T_{ij} = n) = Pr(X_n = s_j, X_{n-1} \neq s_j, \dots, X_1 \neq s_j | X_0 = s_i)$$
 (5)

and can be found recursively using Equation 6, given that  $h_{ij}^{(n)} = p_{ij}$ .

$$h_{ij}^{(n)} = \sum_{k \in S - \{s_j\}} p_{ik} h_{kj}^{(n-1)}.$$
 (6)

If in the definition of the first passage time we let  $s_i = s_j$ , we obtain the first return time  $T_i = \inf\{n \ge 1 : X_n = s_i | X_0 = s_i\}$ . A state  $s_i$  is said to be recurrent if it is visited infinitely often, i.e.,  $Pr(T_i < +\infty | X_0 = s_i) = 1$ . On the opposite,  $s_i$  is called transient if there is a positive probability that the chain will never return to  $s_i$ , i.e.,  $Pr(T_i = +\infty | X_0 = s_i) > 0$ .

Given a time homogeneous Markov chain with transition matrix P, a stationary distribution z is a stochastic row vector such that  $z = z \cdot P$ , where  $0 \le z_j \le 1 \,\forall j$  and  $\sum_j z_j = 1$ .

If a DTMC  $\{X_n\}$  is irreducible and aperiodic, then it has a limit distribution and this distribution is stationary. As a consequence, if P is the  $k \times k$  transition matrix of the chain and  $z = (z_1, ..., z_k)$  is the eigenvector of P such that  $\sum_{i=1}^k z_i = 1$ , then we get

$$\lim_{n \to \infty} P^n = Z,\tag{7}$$

where Z is the matrix having all rows equal to z. The stationary distribution of  $\{X_n\}$  is represented by z.

## 2.3. A short example

Consider the following numerical example. Suppose we have a DTMC with a set of 3 possible states  $S = \{s_1, s_2, s_3\}$ . Let the transition matrix be

$$P = \begin{bmatrix} 0.5 & 0.2 & 0.3 \\ 0.15 & 0.45 & 0.4 \\ 0.25 & 0.35 & 0.4 \end{bmatrix}. \tag{8}$$

In P,  $p_{11} = 0.5$  is the probability that  $X_1 = s_1$  given that we observed  $X_0 = s_1$  is 0.5, and so on. It is easy to see that the chain is irreducible since all the states communicate (it is made by one communicating class only).

Suppose that the current state of the chain is  $X_0 = s_2$ , i.e.,  $x^{(0)} = (010)$ , then the probability distribution of states after 1 and 2 steps can be computed as shown in Equations 9 and 10.

$$x^{(1)} = (0\ 1\ 0) \begin{bmatrix} 0.5 & 0.2 & 0.3 \\ 0.15 & 0.45 & 0.4 \\ 0.25 & 0.35 & 0.4 \end{bmatrix} = (0.15\ 0.45\ 0.4). \tag{9}$$

$$x^{(n)} = x^{(n-1)}P \to (0.15\ 0.45\ 0.4) \begin{bmatrix} 0.5 & 0.2 & 0.3 \\ 0.15 & 0.45 & 0.4 \\ 0.25 & 0.35 & 0.4 \end{bmatrix} = (0.2425\ 0.3725\ 0.385). \tag{10}$$

If, f.e., we are interested in the probability of reaching the state  $s_3$  in two steps, then  $Pr(X_2 = s_3 | X_0 = s_2) = 0.385$ .

# 3. The structure of the package

### 3.1. Creating markovchain objects

The package is loaded within the R command line as follows:

R> library("markovchain")

The markovchain and markovchainList S4 classes (Chambers 2008) are defined within the markovchain package as displayed:

Class "markovchain" [package "markovchain"]

Slots:

Name: states byrow transitionMatrix Class: character logical matrix

Name: name Class: character

Class "markovchainList" [package "markovchain"]

Slots:

Name: markovchains name Class: list character

The first class has been designed to handle homogeneous Markov chain processes, while the latter (which is itself a list of markovchain objects) has been designed to handle non-homogeneous Markov chains processes.

Any element of markovchain class is comprised by following slots:

- 1. states: a character vector, listing the states for which transition probabilities are defined.
- 2. byrow: a logical element, indicating whether transition probabilities are shown by row or by column.
- 3. transitionMatrix: the probabilities of the transition matrix.
- 4. name: optional character element to name the DTMC.

The markovchainList objects are defined by following slots:

- 1. markovchains: a list of markovchain objects.
- 2. name: optional character element to name the DTMC.

The markovchain objects can be created either in a long way, as the following code shows

When new("markovchain") is called alone, a default Markov chain is created.

```
R> defaultMc <- new("markovchain")</pre>
```

The quicker way to create markovchain objects is made possible thanks to the implemented initialize S4 method that checks that:

- the transitionMatrix to be a transition matrix, i.e., all entries to be probabilities and either all rows or all columns to sum up to one.
- the columns and rows names of transitionMatrix to be defined and to coincide with states vector slot.

The markovchain objects can be collected in a list within markovchainList S4 objects as following example shows.

### 3.2. Handling markovchain objects

Table 1 lists which methods handle and manipulate markovchain objects.

The examples that follow shows how operations on markovchain objects can be easily performed. For example, using the previously defined matrix we can find what is the probability distribution of expected weather states in two and seven days, given the actual state to be cloudy.

| Method | Purpose  |
|--------|--|
| *      | Direct multiplication for transition matrices.                       |
| [      | Direct access to the elements of the transition matrix.              |
| ==     | Equality operator between two transition matrices.                   |
| as     | Operator to convert markovchain objects into data.frame and          |
|        | table object.  |
| dim    | Dimension of the transition matrix.                                  |
| names  | Equal to states.   |
| plot   | plot method for markovchain objects.                                 |
| print  | print method for markovchain objects.                                |
| show   | show method for markovchain objects.                                 |
| states | Name of the transition states.                                       |
| t      | Transposition operator (which switches byrow slot value and modifies |
|        | the transition matrix coherently).                                   |

Table 1: markovchain methods for handling markovchain objects.

```
R> initialState <- c(0, 1, 0)
R> after2Days <- initialState * (mcWeather * mcWeather)
R> after7Days <- initialState * (mcWeather ^ 7)
R> after2Days

    sunny cloudy rain
[1,] 0.39 0.355 0.255
R> round(after7Days, 3)

    sunny cloudy rain
[1,] 0.462 0.319 0.219
```

A similar answer could have been obtained defining the vector of probabilities as a column vector. A column - defined probability matrix could be set up either creating a new matrix or transposing an existing markovchain object thanks to the t method.

```
R> initialState <- c(0, 1, 0)
R> after2Days <- (t(mcWeather) * t(mcWeather)) * initialState
R> after7Days <- (t(mcWeather) ^ 7) * initialState
R> after2Days

[,1]
sunny 0.390
cloudy 0.355
rain 0.255

R> round(after7Days, 3)
```

```
[,1]
sunny 0.462
cloudy 0.319
rain 0.219
```

Basic methods have been defined for markovchain objects to quickly get states and transition matrix dimension.

```
R> states(mcWeather)
[1] "sunny" "cloudy" "rain"
R> names(mcWeather)
[1] "sunny" "cloudy" "rain"
R> dim(mcWeather)
[1] 3
```

A direct access to transition probabilities is provided both by transitionProbability method and "[" method.

```
R> transitionProbability(mcWeather, "cloudy", "rain")
[1] 0.3
R> mcWeather[2,3]
```

[1] 0.3

The transition matrix of a markovchain object can be displayed using print or show methods (the latter being less laconic). Similarly, the underlying transition probability diagram can be plotted by the use of plot method (as shown in Figure 1) which is based on **igraph** package (Csardi and Nepusz 2006). plot method for markovchain objects is a wrapper of plot.igraph for igraph S4 objects defined within the **igraph** package. Additional parameters can be passed to plot function to control the network graph layout. There are also **diagram** and **DiagrammeR** ways available for plotting as shown in Figure 2.

### R> print(mcWeather)

```
    sunny
    cloudy
    rain

    sunny
    0.7
    0.20
    0.10

    cloudy
    0.3
    0.40
    0.30

    rain
    0.2
    0.45
    0.35
```

### **Weather transition matrix**

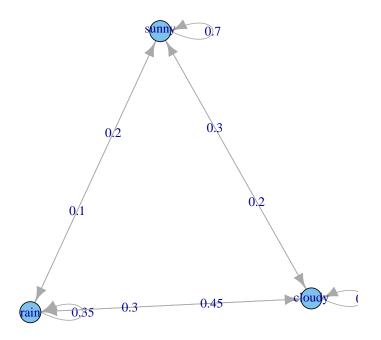


Figure 1: Weather example. Markov chain plot.

### R> show(mcWeather)

### Weather

 ${\tt A}$   ${\tt 3}$  - dimensional discrete Markov Chain with following states sunny cloudy rain

The transition matrix (by rows) is defined as follows sunny cloudy rain

sunny 0.7 0.20 0.10
cloudy 0.3 0.40 0.30
rain 0.2 0.45 0.35

Import and export from some specific classes is possible, as shown in Figure 3 and in the following code.

R> mcDf <- as(mcWeather, "data.frame")</pre>



Figure 2: Weather example. Markov chain plot with diagram. plot (mcWeather, package="diagram", box.size = 0.04)

```
R> mcNew <- as(mcDf, "markovchain")</pre>
R> mcDf
             t1 prob
      t0
1 sunny sunny 0.70
2 sunny cloudy 0.20
3 sunny
         rain 0.10
4 cloudy sunny 0.30
5 cloudy cloudy 0.40
6 cloudy
          rain 0.30
   rain sunny 0.20
7
  rain cloudy 0.45
8
           rain 0.35
  {\tt rain}
R> mcIgraph <- as(mcWeather, "igraph")</pre>
R> library(msm)
R > Q \leftarrow rbind (c(0, 0.25, 0, 0.25),
                c(0.166, 0, 0.166, 0.166),
                c(0, 0.25, 0, 0.25),
+
                c(0, 0, 0, 0))
R> cavmsm <- msm(state ~ years, subject = PTNUM, data = cav, qmatrix = Q, death = 4)
R> msmMc <- as(cavmsm, "markovchain")</pre>
R> msmMc
Unnamed Markov chain
 A 4 - dimensional discrete Markov Chain with following states
 State 1 State 2 State 3 State 4
 The transition matrix
                         (by rows) is defined as follows
            State 1
                       State 2
                                  State 3
                                             State 4
State 1 0.853958721 0.08836953 0.01475543 0.04291632
State 2 0.155576908 0.56663284 0.20599563 0.07179462
State 3 0.009903994 0.07853691 0.65965727 0.25190183
R> library(etm)
R> data(sir.cont)
R> sir.cont <- sir.cont[order(sir.cont$id, sir.cont$time), ]</pre>
R> for (i in 2:nrow(sir.cont)) {
     if (sir.cont$id[i]==sir.cont$id[i-1]) {
       if (sir.cont$time[i]==sir.cont$time[i-1]) {
         sir.conttime[i-1] <- sir.conttime[i-1] - 0.5
       }
     }
+
R> tra <- matrix(ncol=3,nrow=3,FALSE)</pre>
R> tra[1, 2:3] <- TRUE</pre>
R > tra[2, c(1, 3)] < - TRUE
```

```
R> tr.prob <- etm(sir.cont, c("0", "1", "2"), tra, "cens", 1)
R> tr.prob
Multistate model with 2 transient state(s)
 and 1 absorbing state(s)
Possible transitions:
 from to
    0 1
    0 2
    1 0
    1 2
Estimate of P(1, 183)
  0 1 2
0 0 0 1
1 0 0 1
2001
Estimate of cov(P(1, 183))
    0 0 1 0 2 0 0 1 1 1 2 1
                                      0 2
                                                     1 2 2 2
                          0 0.000000e+00 0.000000e+00
0 0
      0
          0
              0
                  0
                      0
                                                           0
                          0 0.000000e+00 0.000000e+00
1 0
          0
      0
              0
                  0
                      0
                                                           0
2 0
              0
                          0 0.000000e+00 0.000000e+00
                         0 0.000000e+00 0.000000e+00
0 1
      0
          0
              0
                  0
                      0
                                                           0
                         0 0.000000e+00 0.000000e+00
1 1
      0
          0
              0
                  0
                      0
                                                           0
2 1
                         0 0.000000e+00 0.000000e+00
      0
          0
              0
                  0
                      0
                                                           0
0 2
      0
          0
              0
                  0
                      0
                         0 -2.864030e-20 -1.126554e-19
                                                           0
1 2
                         0 -4.785736e-20 2.710505e-19
      0
          0
              0
                  0
                      0
                                                           0
                          0 0.000000e+00 0.000000e+00
2 2
      0
          0
              0
                      0
R> etm2mc<-as(tr.prob, "markovchain")</pre>
R> etm2mc
Unnamed Markov chain
 A 3 - dimensional discrete Markov Chain with following states
 0 1 2
 The transition matrix
                         (by rows)
                                    is defined as follows
          0
                    1
0 0.0000000 0.5000000 0.5000000
1 0.5000000 0.0000000 0.5000000
2 0.3333333 0.3333333 0.3333333
```

Coerce from matrix method, as the code below shows, represents another approach to create a markovchain method starting from a given squared probability matrix.

# Import – Export from and to markovchain objects

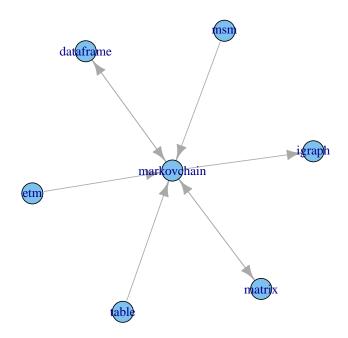


Figure 3: The **markovchain** methods for import and export.

```
R> myMatr<-matrix(c(.1,.8,.1,.2,.6,.2,.3,.4,.3), byrow=TRUE, ncol=3)
R> myMc<-as(myMatr, "markovchain")
R> myMc

Unnamed Markov chain
   A 3 - dimensional discrete Markov Chain with following states
   s1 s2 s3
   The transition matrix (by rows) is defined as follows
        s1 s2 s3
s1 0.1 0.8 0.1
s2 0.2 0.6 0.2
s3 0.3 0.4 0.3
```

Non-homogeneous Markov chains can be created with the aid of markovchainList object. The example that follows arises from health insurance, where the costs associated to patients in a Continuous Care Health Community (CCHC) are modelled by a non-homogeneous Markov Chain, since the transition probabilities change by year. Methods explicitly written for markovchainList objects are: print, show, dim and [.

```
Continuous Care Health Community list of Markov chain(s)
Markovchain 1
state t0
 A 3 - dimensional discrete Markov Chain with following states
 H I D
 The transition matrix
                         (by rows) is defined as follows
        Ι
    Η
H 0.7 0.2 0.1
I 0.1 0.6 0.3
D 0.0 0.0 1.0
Markovchain 2
state t1
 A 3 - dimensional discrete Markov Chain with following states
 H I D
 The transition matrix
                         (by rows) is defined as follows
    Η
       Ι
           D
H 0.5 0.3 0.2
I 0.0 0.4 0.6
D 0.0 0.0 1.0
Markovchain 3
state t2
 A 3 - dimensional discrete Markov Chain with following states
 H I D
 The transition matrix (by rows) is defined as follows
    Н
       Ι
H 0.3 0.2 0.5
```

```
I 0.0 0.2 0.8
D 0.0 0.0 1.0

Markovchain 4
state t3
A 3 - dimensional discrete Markov Chain with following states
H I D

The transition matrix (by rows) is defined as follows
H I D
H 0 0 1
I 0 0 1
D 0 0 1
```

It is possible to perform direct access to markovchainList elements, as well as to determine the number of markovchain objects by which a markovchainList object is composed.

```
R> mcCCRC[[1]]
state t0
A 3 - dimensional discrete Markov Chain with following states
H I D
The transition matrix (by rows) is defined as follows
H I D
H 0.7 0.2 0.1
I 0.1 0.6 0.3
D 0.0 0.0 1.0
R> dim(mcCCRC)
```

[1] 4

The markovchain package contains some data found in the literature related to DTMC models (see Section 6). Table 2 lists datasets and tables included within the current release of the package.

| Dataset        | Description   |
|----------------|---|
| blanden        | Mobility across income quartiles, Jo Blanden and Machin (2005).   |
| craigsendi     | CD4 cells, B. A. Craig and A. A. Sendi (2002).                    |
| preproglucacon | Preproglucacon DNA basis, P. J. Avery and D. A. Henderson (1999). |
| rain           | Alofi Island rains, P. J. Avery and D. A. Henderson (1999).       |
| holson         | Individual states trajectiories.                                  |

Table 2: The markovchain data.frame and table.

Finally, Table 3 lists the demos included in the demo directory of the package.

| Dataset              | Description  |
|----------------------|--|
| bard.R               | Structural analysis of Markov chains from Bard PPT.  |
| examples.R           | Notable Markov chains, e.g., The Gambler Ruin chain. |
| ${\tt quickStart.R}$ | Generic examples.                                    |

Table 3: The markovchain demos.

# 4. Probability with markovchain objects

The markovchain package contains functions to analyse DTMC from a probabilistic perspective. For example, the package provides methods to find stationary distributions and identifying absorbing and transient states. Many of these methods come from MATLAB listings that have been ported into R. For a full description of the underlying theory and algorithm the interested reader can overview the original MATLAB listings, Feres (2007) and Montgomery (2009).

Table 4 shows methods that can be applied on markovchain objects to perform probabilistic analysis.

| Method                       | Returns  |
|------------------------------|--|
| absorbingStates              | the absorbing states of the transition matrix, if any. |
| ${	t steadyStates}$          | the vector(s) of steady state(s) in matrix form.       |
| ${\tt communicatingClasses}$ | list of communicating classes.                         |
|                              | $s_j$ , given actual state $s_i$ .                     |
| canonicForm                  | the transition matrix into canonic form.               |
| is.accessible                | verification if a state j is reachable from state i.   |
| is.irreducible               | verification whether a DTMC is irreducible.            |
| period                       | the period of an irreducible DTMC.                     |
| recurrentClasses             | list of recurrent classes.                             |
| ${	t steadyStates}$          | the vector(s) of steady state(s) in matrix form.       |
| summary                      | DTMC summary.  |
| transientStates              | the transient states of the transition matrix, if any. |

Table 4: markovchain methods: statistical operations.

The conditional distribution of weather states, given that current day's weather is sunny, is given by following code.

R> conditionalDistribution(mcWeather, "sunny")

```
sunny cloudy rain 0.7 0.2 0.1
```

The steady state(s), also known as stationary distribution(s), of the Markov chains are identified by the such described algorithm:

- 1. decompose the transition matrix in eigenvalues and eigenvectors;
- 2. consider only eigenvectors corresponding to eigenvalues equal to one;
- 3. normalize such eigenvalues so that the sum of their components is one.

The result is returned in matrix form.

R> steadyStates(mcWeather)

```
sunny cloudy rain [1,] 0.4636364 0.3181818 0.2181818
```

It is possible for a Markov chain to have more than one stationary distribution, as the gambler ruin example shows.

```
R> gamblerRuinMarkovChain <- function(moneyMax, prob = 0.5) {</pre>
     require(matlab)
     matr <- zeros(moneyMax + 1)</pre>
     states <- as.character(seq(from = 0, to = moneyMax, by = 1))
     rownames(matr) = states; colnames(matr) = states
     matr[1,1] = 1; matr[moneyMax + 1, moneyMax + 1] = 1
     for(i in 2:moneyMax)
     { matr[i,i-1] = 1 - prob; matr[i, i + 1] = prob }
     out <- new("markovchain",</pre>
              transitionMatrix = matr,
               name = paste("Gambler ruin", moneyMax, "dim", sep = " ")
     return(out)
+
R> mcGR4 <- gamblerRuinMarkovChain(moneyMax = 4, prob = 0.5)
R> steadyStates(mcGR4)
     0 1 2 3 4
[1,] 1 0 0 0 0
[2,] 0 0 0 0 1
Absorbing states are determined by means of absorbingStates method.
R> absorbingStates(mcGR4)
[1] "0" "4"
R> absorbingStates(mcWeather)
character(0)
The key function used within Feres (2007) (and markovchain's derived functions) is
.commclassKernel, that is called below.
```

```
R> .commclassesKernel <- function(P){
+          m <- ncol(P)
+          stateNames <- rownames(P)
+          T <- zeros(m)
+          i <- 1
+          while (i <= m) {</pre>
```

```
+
                        a <- i
                        b \leftarrow zeros(1,m)
                        b[1,i] <-1
                        old <- 1
                       new <- 0
                        while (old != new) {
                                  old \leftarrow sum(find(b > 0))
                                  n \leftarrow size(a)[2]
                                  matr <- matrix(as.numeric(P[a,]), ncol = m,</pre>
                                  c <- colSums(matr)</pre>
                                  d \leftarrow find(c)
                                  n \leftarrow size(d)[2]
                                  b[1,d] <- ones(1,n)
                                 new <- sum(find(b>0))
                                  a <- d
                        }
                        T[i,] \leftarrow b
                        i <- i+1 }
             F \leftarrow t(T)
             C \leftarrow (T > 0)&(F > 0)
             v \leftarrow (apply(t(C) == t(T), 2, sum) == m)
             colnames(C) <- stateNames</pre>
             rownames(C) <- stateNames
             names(v) <- stateNames</pre>
             out \leftarrow list(C = C, v = v)
             return(out)
  }
```

The .commclassKernel function gets a transition matrix of dimension n and return a list of two items:

- 1. C, an adjacency matrix showing for each state  $s_j$  (in the row) which states lie in the same communicating class of  $s_j$  (flagged with 1).
- 2. v, a binary vector indicating whether the state  $s_j$  is transient (0) or not (1).

These functions are used by two other internal functions on which the summary method for markovchain objects works.

The example matrix used in Feres (2007) well exemplifies the purpose of the function.

```
R> P <- matlab::zeros(10)
R> P[1, c(1, 3)] <- 1/2;
R> P[2, 2] <- 1/3; P[2,7] <- 2/3;
R> P[3, 1] <- 1;
R> P[4, 5] <- 1;
R> P[5, c(4, 5, 9)] <- 1/3;
```

```
R > P[6, 6] < -1;
R> P[7, 7] <- 1/4; P[7,9] <- 3/4;
R > P[8, c(3, 4, 8, 10)] < -1/4;
R> P[9, 2] <- 1;
R > P[10, c(2, 5, 10)] < -1/3;
R> rownames(P) <- letters[1:10]</pre>
R> colnames(P) <- letters[1:10]</pre>
R> probMc <- new("markovchain", transitionMatrix = P,</pre>
                name = "Probability MC")
R> .commclassesKernel(P)
$C
                 С
                       d
                                   f
                                              h
                             е
                                         g
a TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
b FALSE TRUE FALSE FALSE FALSE TRUE FALSE TRUE FALSE
  TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
d FALSE FALSE FALSE TRUE TRUE FALSE FALSE FALSE FALSE
e FALSE FALSE FALSE TRUE TRUE FALSE FALSE FALSE FALSE
f FALSE FALSE FALSE FALSE TRUE FALSE FALSE FALSE FALSE
g FALSE TRUE FALSE FALSE FALSE
                                     TRUE FALSE TRUE FALSE
h FALSE FALSE FALSE FALSE FALSE FALSE
                                           TRUE FALSE FALSE
i FALSE TRUE FALSE FALSE FALSE
                                     TRUE FALSE
j FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE TRUE
$v
   а
                           е
                                 f
      TRUE TRUE FALSE FALSE TRUE TRUE FALSE TRUE FALSE
R> summary(probMc)
Probability MC Markov chain that is composed by:
Closed classes:
a c
bgi
Recurrent classes:
{a,c},{b,g,i},{d,e},{f}
Transient classes:
\{d,e\},\{h\},\{j\}
The Markov chain is not irreducible
The absorbing states are: f
```

All states that pertain to a transient class are named "transient" and a specific method has been written to elicit them.

### R> transientStates(probMc)

```
[1] "d" "e" "h" "j"
```

Listings from Feres (2007) have been adapted into canonicForm method that turns a Markov chain into canonic form.

```
R> probMcCanonic <- canonicForm(probMc)</pre>
R> probMc
Probability MC
A 10 - dimensional discrete Markov Chain with following states
abcdefghij
The transition matrix
                 (by rows)
                         is defined as follows
                    d
                           e f
d 0.0 0.0000000 0.00 0.0000000 1.0000000 0 0.0000000 0.00 0.0000000
e 0.0 0.0000000 0.00 0.3333333 0.3333333 0 0.0000000 0.00 0.3333333
f 0.0 0.0000000 0.00 0.0000000 0.0000000 1 0.0000000 0.00 0.0000000
h 0.0 0.0000000 0.25 0.2500000 0.0000000 0 0.0000000 0.25 0.0000000
j 0.0 0.3333333 0.00 0.0000000 0.3333333 0 0.0000000 0.00 0.0000000
a 0.0000000
b 0.0000000
c 0.0000000
d 0.0000000
e 0.0000000
f 0.000000
g 0.0000000
h 0.2500000
i 0.0000000
j 0.3333333
R> probMcCanonic
Probability MC
A 10 - dimensional discrete Markov Chain with following states
```

```
acbgifdehj
The transition matrix
               (by rows)
                     is defined as follows
           b
                       i f
b 0.0 0.00 0.3333333 0.6666667 0.0000000 0 0.0000000 0.0000000 0.00
g 0.0 0.00 0.0000000 0.2500000 0.7500000 0 0.0000000 0.0000000 0.00
```

```
f 0.0 0.00 0.0000000 0.0000000 0.0000000 1 0.0000000 0.0000000 0.00
e 0.0 0.00 0.0000000 0.0000000 0.3333333 0 0.3333333 0.3333333 0.00
h 0.0 0.25 0.0000000 0.0000000 0.0000000 0 0.2500000 0.0000000 0.25
j 0.0 0.00 0.3333333 0.0000000 0.0000000 0 0.0000000 0.3333333 0.00
a 0.0000000
c 0.0000000
b 0.0000000
g 0.0000000
i 0.000000
f 0.000000
d 0.0000000
e 0.0000000
h 0.2500000
j 0.3333333
```

The function is.accessible permits to investigate whether a state  $s_j$  is accessible from state  $s_i$ , that is whether the probability to eventually reach  $s_j$  starting from  $s_i$  is greater than zero.

```
R> is.accessible(object = probMc, from = "a", to = "c")
[1] TRUE
R> is.accessible(object = probMc, from = "g", to = "c")
[1] FALSE
```

In Section 2.2 we observed that, if a DTMC is irreducible, all its states share the same periodicity. Then, the period function returns the periodicity of the DTMC, provided that it is irreducible. The example that follows shows how to find if a DTMC is reducible or irreducible by means of the function is.irreducible and, in the latter case, the method period is used to compute the periodicity of the chain.

```
R> E <- matrix(0, nrow = 4, ncol = 4)

R> E[1, 2] <- 1

R> E[2, 1] <- 1/3; E[2, 3] <- 2/3

R> E[3,2] <- 1/4; E[3, 4] <- 3/4

R> E[4, 3] <- 1

R> mcE <- new("markovchain", states = c("a", "b", "c", "d"), transitionMatrix = E, the name = "E")

R> is.irreducible(mcE)
```

[1] TRUE

```
R> period(mcE)
```

### [1] 2

The example Markov chain found in Mathematica web site (Wolfram Research 2013a) has been used, and is plotted in Figure 4.

```
R> require(matlab)
R> mathematicaMatr <- zeros(5)</pre>
R> mathematicaMatr[1,] <- c(0, 1/3, 0, 2/3, 0)
R> mathematicaMatr[2,] <- c(1/2, 0, 0, 0, 1/2)
R> mathematicaMatr[3,] <- c(0, 0, 1/2, 1/2, 0)
R> mathematicaMatr[4,] <- c(0, 0, 1/2, 1/2, 0)
R > mathematicaMatr[5,] <- c(0, 0, 0, 0, 1)
R> statesNames <- letters[1:5]</pre>
R> mathematicaMc <- new("markovchain", transitionMatrix = mathematicaMatr,
                       name = "Mathematica MC", states = statesNames)
Mathematica MC Markov chain that is composed by:
Closed classes:
c d
Recurrent classes:
\{c,d\},\{e\}
Transient classes:
\{a,b\}
The Markov chain is not irreducible
The absorbing states are: e
```

Feres (2007) provides code to compute first passage time (within 1, 2, ..., n steps) given the initial state to be i. The MATLAB listings translated into R on which the firstPassage function is based are

```
R> .firstpassageKernel <- function(P, i, n){
+    G <- P
+    H <- P[i,]
+    E <- 1 - diag(size(P)[2])
+    for (m in 2:n) {
+       G <- P %*% (G * E)
+      H <- rbind(H, G[i,])
+    }
+    return(H)
+ }</pre>
```

We conclude that the probability for the first rainy day to be the third one, given that the current state is sunny, is given by

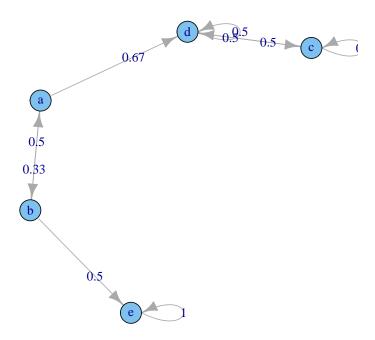


Figure 4: Mathematica 9 example. Markov chain plot.

```
R> firstPassagePdF <- firstPassage(object = mcWeather, state = "sunny",
                                    n = 10)
R> firstPassagePdF[3, 3]
[1] 0.121
```

# 5. Statistical analysis

Table 5 lists the functions and methods implemented within the package which help to fit, simulate and predict DTMC.

| Function       | Purpose   |
|----------------|---|
| markovchainFit | Function to return fitted Markov chain for a given sequence.    |
| predict        | Method to calculate predictions from markovchain or             |
|                | markovchainList objects.  |
| rmarkovchain   | Function to sample from markovchain or markovchainList objects. |

Table 5: The **markovchain** statistical functions.

### 5.1. Simulation

2

3

1

1

Ι

Simulating a random sequence from an underlying DTMC is quite easy thanks to the function rmarkovchain. The following code generates a year of weather states according to mcWeather underlying stochastic process.

```
R> weathersOfDays <- rmarkovchain(n = 365, object = mcWeather, t0 = "sunny")
R> weathersOfDays[1:30]
```

```
[1] "sunny"
                                                     "cloudy" "cloudy"
              "sunny"
                        "sunny"
                                 "sunny"
                                           "sunny"
 [8] "sunny"
              "sunny"
                        "sunny"
                                 "sunny"
                                           "cloudy" "rain"
                                                              "rain"
[15] "cloudy" "rain"
                        "rain"
                                 "rain"
                                           "rain"
                                                     "sunny"
                                                              "sunny"
[22] "sunny"
                                 "cloudy" "sunny"
                                                     "cloudy" "rain"
              "sunny"
                        "rain"
[29] "cloudy" "sunny"
```

Similarly, it is possible to simulate one or more sequences from a non-homogeneous Markov chain, as the following code (applied on CCHC example) exemplifies.

```
R> patientStates <- rmarkovchain(n = 5, object = mcCCRC, t0 = "H",
                                  include.t0 = TRUE)
R> patientStates[1:10,]
   iteration values
1
           1
                  Η
                  Η
```

| 4      | 1 | D |
|--------|---|---|
| 5      | 1 | D |
| 6      | 2 | Н |
| 7      | 2 | Н |
| 8<br>9 | 2 | Н |
| 9      | 2 | Н |
| 10     | 2 | D |

### 5.2. Estimation

A time homogeneous Markov chain can be fit from given data. Four methods have been implemented within current version of **markovchain** package: maximum likelihood, maximum likelihood with Laplace smoothing, Bootstrap approach, maximum a posteriori.

Equation 11 shows the maximum likelihood estimator (MLE) of the  $p_{ij}$  entry, where the  $n_{ij}$  element consists in the number sequences  $(X_t = s_i, X_{t+1} = s_j)$  found in the sample, that is

$$\hat{p}_{ij}^{MLE} = \frac{n_{ij}}{\sum_{u=1}^{k} n_{iu}}.$$
(11)

Equation 12 shows the standardError of the MLE (Skuriat-Olechnowska 2005).

$$SE_{ij} = \frac{\hat{p}_{ij}^{MLE}}{\sqrt{n_{ij}}} \tag{12}$$

Weather MLE

A 3 - dimensional discrete Markov Chain with following states cloudy rain sunny
The transition matrix (by rows) is defined as follows

The transition matrix (by rows) is defined as follows cloudy rain sunny

cloudy 0.4444444 0.2936508 0.2619048

rain 0.4691358 0.3333333 0.1975309

sunny 0.2101911 0.1082803 0.6815287

R> weatherFittedMLE\$standardError

```
cloudy rain sunny cloudy 0.05939139 0.04827589 0.04559177 rain 0.07610388 0.06415003 0.04938272 sunny 0.03658957 0.02626182 0.06588586
```

The Laplace smoothing approach is a variation of the MLE, where the  $n_{ij}$  is substituted by  $n_{ij} + \alpha$  (see Equation 13), being  $\alpha$  an arbitrary positive stabilizing parameter.

$$\hat{p}_{ij}^{LS} = \frac{n_{ij} + \alpha}{\sum\limits_{u=1}^{k} (n_{iu} + \alpha)}$$
(13)

```
Weather LAPLACE
```

A 3 - dimensional discrete Markov Chain with following states cloudy rain sunny

The transition matrix (by rows) is defined as follows cloudy rain sunny cloudy 0.4444180 0.2936602 0.2619218 rain 0.4690855 0.3333333 0.1975811 sunny 0.2102146 0.1083233 0.6814621

Both MLE and Laplace approach are based on the createSequenceMatrix functions that converts a data (character) sequence into a contingency table, showing the  $(X_t = i, X_{t+1} = j)$  distribution within the sample, as code below shows.

R> createSequenceMatrix(stringchar = weathersOfDays)

```
cloudy rain sunny
cloudy 56 37 33
rain 38 27 16
sunny 33 17 107
```

An issue occurs when the sample contains only one realization of a state (say  $X_{\beta}$ ) which is located at the end of the data sequence, since it yields to a row of zero (no sample to estimate the conditional distribution of the transition). In this case the estimated transition matrix is corrected assuming  $p_{\beta,j} = 1/k$ , being k the possible states.

A bootstrap estimation approach has been developed within the package in order to provide an indication of the variability of  $\hat{p}_{ij}$  estimates. The bootstrap approach implemented within the **markovchain** package follows these steps:

- 1. bootstrap the data sequences following the conditional distributions of states estimated from the original one. The default bootstrap samples is 10, as specified in nboot parameter of markovchainFit function.
- 2. apply MLE estimation on bootstrapped data sequences that are saved in bootStrapSamples slot of the returned list.

3. the  $p^{BOOTSTRAP}_{ij}$  is the average of all  $p^{MLE}_{ij}$  across the bootStrapSamples list, normalized by row. A standardError of  $p^{M\hat{L}E}_{ij}$  estimate is provided as well.

BootStrap Estimate

 ${\tt A}$  - dimensional discrete Markov Chain with following states cloudy rain sunny

The transition matrix (by rows) is defined as follows

cloudy rain sunny

cloudy 0.4420864 0.2949811 0.2629325

rain 0.4721776 0.3343147 0.1935077

sunny 0.2066387 0.1112359 0.6821254

R> weatherFittedB00T\$standardError

```
cloudy rain sunny cloudy 0.004496236 0.004389933 0.003324478 rain 0.005973287 0.005042829 0.004190635 sunny 0.003152474 0.002496065 0.003877712
```

The bootstrapping process can be done in parallel.

R> weatherFittedB00TParallel\$standardError

The parallel bootstrapping uses all the available cores on a machine by default. However, it is also possible to tune the number of threads used. Note that this should be done in R before calling the markovchainFit function. For example, the following code will set the number of threads to 4.

R> RcppParallel::setNumThreads(4)

For more details, please refer to **RcppParallel** (http://rcppcore.github.io/RcppParallel/). For all the fitting methods, the logLikelihood (Skuriat-Olechnowska 2005) denoted in Equation 14 is provided.

$$LLH = \sum_{i,j} n_{ij} * log(p_{ij})$$
(14)

where  $n_{ij}$  is the entry of the frequency matrix and  $p_{ij}$  is the entry of the transition probability matrix.

### R> weatherFittedMLE\$logLikelihood

[1] -349.6247

### R> weatherFittedB00T\$logLikelihood

### [1] -349.6415

Confidence matrices of estimated parameters (parametric for MLE, non - parametric for BootStrap) are available as well. The confidenceInterval is provided with the two matrices: lowerEndpointMatrix and upperEndpointMatrix. The confidence level (CL) is 0.95 by default and can be given as an argument of the function markovchainFit. This is used to obtain the standard score (z-score). Equations 15 and 16 (Skuriat-Olechnowska 2005) show the confidenceInterval of a fitting. Note that each entry of the matrices is bounded between 0 and 1.

$$LowerEndpoint_{ij} = p_{ij} - zscore(CL) * SE_{ij}$$
(15)

$$UpperEndpoint_{ij} = p_{ij} + zscore(CL) * SE_{ij}$$
(16)

### R> weatherFittedMLE\$confidenceInterval

### \$confidenceLevel

[1] 0.95

# \$lowerEndpointMatrix

cloudy rain sunny cloudy 0.3467543 0.21424402 0.1869130 rain 0.3439561 0.22781592 0.1163035 sunny 0.1500066 0.06508341 0.5731561

# \$upperEndpointMatrix

cloudy rain sunny cloudy 0.5421346 0.3730576 0.3368965 rain 0.5943155 0.4388507 0.2787582 sunny 0.2703756 0.1514771 0.7899013

### R> weatherFittedB00T\$confidenceInterval

# \$confidenceLevel [1] 0.95

# \$lowerEndpointMatrix

cloudy rain sunny cloudy 0.4346908 0.2877603 0.2574642 rain 0.4623524 0.3260200 0.1866148

```
sunny 0.2014534 0.1071302 0.6757471
```

### \$upperEndpointMatrix

```
cloudy rain sunny cloudy 0.4494821 0.3022019 0.2684007 rain 0.4820028 0.3426094 0.2004007 sunny 0.2118241 0.1153415 0.6885037
```

A special function, multinomialConfidenceIntervals, has been written in order to obtain multinomial wise confidence intervals. The code has been based on and Rcpp translation of package's MultinomialCI functions Villacorta (2012) that were themselves based on the Sison and Glaz (1995) paper.

### \$confidenceLevel

[1] 0.95

### \$lowerEndpointMatrix

```
cloudy rain sunny
cloudy 0.3571429 0.20634921 0.17460317
rain 0.3580247 0.22222222 0.08641975
sunny 0.1401274 0.03821656 0.61146497
```

### \$upperEndpointMatrix

```
cloudy rain sunny cloudy 0.5429844 0.3921908 0.3604447 rain 0.5844847 0.4486823 0.3128798 sunny 0.2828687 0.1809579 0.7542063
```

The functions for fitting DTMC have mostly been rewritten in C++ using Rcpp Eddelbuettel (2013) since version 0.2.

Is is also possible to fit a DTMC or a markovchainList object from matrix or data.frame objects as shown in following code.

```
R> data(holson)
R> singleMc<-markovchainFit(data=holson[,2:12],name="holson")
R> mcListFit<-markovchainListFit(data=holson[,2:12],name="holson")
R> mcListFit$estimate[[1]]

time1
A 3 - dimensional discrete Markov Chain with following states
1 2 3
```

```
The transition matrix (by rows) is defined as follows

1 2 3
1 0.94609164 0.05390836 0.0000000
2 0.26356589 0.62790698 0.1085271
3 0.02325581 0.18604651 0.7906977
```

The maximum a posteriori method (MAP) has been implemented using Bayesian inference (Strelioff, Crutchfield, and Hubler 2007). For details on usage, refer to the stand-alone vignette for MAP (Yalamanchi and Spedicato 2015).

### 5.3. Prediction

The *n*-step forward predictions can be obtained using the **predict** methods explicitly written for **markovchain** and **markovchainList** objects. The prediction is the mode of the conditional distribution of  $X_{t+1}$  given  $X_t = s_j$ , being  $s_j$  the last realization of the DTMC (homogeneous or non-homogeneous).

Predicting from a markovchain object

The 3-days forward predictions from markovchain object can be generated as follows, assuming that the last two days were respectively "cloudy" and "sunny".

Predicting from a markovchainList object

Given an initial two year Healty status, the 5-year ahead prediction of any CCRC guest is

```
R> predict(mcCCRC, newdata = c("H", "H"), n.ahead = 5)
[1] "H" "D" "D"
```

The prediction has stopped at time sequence since the underlying non-homogeneous Markov chain has a length of four. In order to continue five years ahead, the continue=TRUE parameter setting makes the predict method keeping to use the last markovchain in the sequence list.

```
R> predict(mcCCRC, newdata = c("H", "H"), n.ahead = 5, continue = TRUE)

[1] "H" "D" "D" "D" "D"
```

### 5.4. Statistical Tests

In this section, we describe the statistical tests: assessing the Markov property (verifyMarkovProperty), the order (assessOrder), the statinarity (assessStationarity) of a Markov chain sequence,

and the divergence test for empirically estimated transition matrices (divergenceTest). For the first three tests, we use the  $\chi^2$  statistics (Anderson and Goodman 1957; Skuriat-Olechnowska 2005). As an example, we use the following sequence.

Assessing the Markov property of a Markov chain sequence

The verifyMarkovProperty function invloves verifying whether the given chain holds the Markov property for which the future state is independent of the past states and depends only on the current state.

$$\Pr\left\{X_{t+1} = m | X_t = j, X_{t-1} = i\right\} = \Pr\left\{X_{t+1} = m | X_t = j\right\}$$
(17)

We first construct a contingency table in which the columns are the frequency of past—present—future (PPF) (or state transition sequence (STS)), present—future (PF) (or two-state occurrences (STO)) and (PF - PPF), and the rows are the possible three state transitions as shown in Table 6 for each possible present to future transition.

| Transitions $(p \rightarrow p \rightarrow f)$ | $PPF (p \rightarrow p \rightarrow f)$ | $PF (p \rightarrow f)$               | PF - PPF |
|---|---------------------------------------|--------------------------------------|----------|
| $a \rightarrow a \rightarrow b$               | $2 (a \rightarrow a \rightarrow b)$   | 4 (a→a)                              | 2        |
| $b \to a \to b$                               | $2 (b \to a \to b)$                   | $5 \text{ (b} \rightarrow \text{a)}$ | 3        |

Table 6: Contingency table for Markov property of the transition from the present state a to the future state b  $(a \rightarrow b)$ .

Using the table, the function performs the  $\chi^2$  test by calling the chisq.test function. This test returns a list of the chi-squared value, the degrees of freedom, and the p-value for each possible transition. If the p-value is greater than the given significance level, we cannot reject the hypothesis that the Markov property holds for the specific transition.

### R> verifyMarkovProperty(sequence)

\$aa
\$aa\$statistic
X-squared
0

\$aa\$parameter
df

1

\$aa\$p.value
[1] 1

\$aa\$method

# [1] "Pearson's Chi-squared test with Yates' continuity correction" \$aa\$data.name [1] "table" \$aa\$observed SSO TSO-SSO 2 \$aa\$expected SSO TSO-SSO a 1.777778 2.222222 b 2.222222 2.777778 \$aa\$residuals SSO TSO-SSO a 0.1666667 -0.1490712 b -0.1490712 0.1333333 \$aa\$stdres SSO TSO-SSO a 0.3 -0.3 b -0.3 0.3 \$aa\$table SSO TSO a 2 4 b 2 5 \$ab \$ab\$statistic X-squared \$ab\$parameter df 1 \$ab\$p.value [1] 1

\$ab\$method

[1] "Pearson's Chi-squared test with Yates' continuity correction"

\$ab\$data.name

```
[1] "table"
```

### \$ab\$observed

SSO TSO-SSO

a 2 2

b 2 3

# \$ab\$expected

SSO TSO-SSO

a 1.777778 2.222222

b 2.222222 2.777778

# \$ab\$residuals

SSO TSO-SSO

a 0.1666667 -0.1490712

b -0.1490712 0.1333333

### \$ab\$stdres

SSO TSO-SSO

a 0.3 -0.3

b -0.3 0.3

### \$ab\$table

SSO TSO

a 2 4

b 2 5

## \$ba

\$ba\$statistic

X-squared

1.55307e-31

# \$ba\$parameter

df

1

# \$ba\$p.value

[1] 1

### \$ba\$method

[1] "Pearson's Chi-squared test with Yates' continuity correction"

### \$ba\$data.name

[1] "table"

## \$ba\$observed

SSO TSO-SSO

```
4
            1
b
   1
            1
$ba$expected
       SSO
             TSO-SSO
a 3.571429 1.4285714
b 1.428571 0.5714286
$ba$residuals
         SSO
                TSO-SSO
a 0.2267787 -0.3585686
b -0.3585686 0.5669467
$ba$stdres
         SSO
                TSO-SSO
a 0.7937254 -0.7937254
b -0.7937254 0.7937254
$ba$table
 SSO TSO
  4
       5
        2
    1
$bb
$bb$statistic
 X-squared
1.55307e-31
$bb$parameter
df
 1
$bb$p.value
[1] 1
$bb$method
[1] "Pearson's Chi-squared test with Yates' continuity correction"
$bb$data.name
[1] "table"
$bb$observed
  SSO TSO-SSO
  1
  1
            1
```

### \$bb\$expected

SSO TSO-SSO a 1.4285714 3.571429 b 0.5714286 1.428571

### \$bb\$residuals

SSO TSO-SSO a -0.3585686 0.2267787 b 0.5669467 -0.3585686

### \$bb\$stdres

SSO TSO-SSO a -0.7937254 0.7937254 b 0.7937254 -0.7937254

### \$bb\$table

SSO TSO a 1 5 b 1 2

Assessing the order of a Markov chain sequence

The assessOrder function checks whether the given chain is of first order or of second order. For each possible present state, we construct a contingency table of the frequency of the future state for each past to present state transition as shown in Table 7.

| past | present | future | future |
|------|---------|--------|--------|
|      |         | a      | b      |
| a    | a       | 2      | 2      |
| b    | a       | 2      | 2      |

Table 7: Contingency table to assess the order for the present state a.

Using the table, the function performs the  $\chi^2$  test by calling the **chisq.test** function. This test returns a list of the chi-squared value and the p-value. If the p-value is greater than the given significance level, we cannot reject the hypothesis that the sequence is of first order.

R> data(rain)
R> assessOrder(rain\$rain)

\$statistic [1] 26.09575

\$p.value

[1] 0.01040395

Assessing the stationarity of a Markov chain sequence

The assessStationarity function assesses if the transition probabilities of the given chain change over time. To be more specific, the chain is stationary if the following condition meets.

$$p_{ij}(t) = p_{ij} \quad \text{for all} \quad t \tag{18}$$

For each possible state, we construct a contingency table of the estimated transition probabilities over time as shown in Table 8.

| time (t) | probability of transition to a | probability of transition to b |
|----------|--------------------------------|--------------------------------|
| 1        | 0                              | 1                              |
| 2        | 0                              | 1                              |
|          |                                |                                |
| •        |                                | •                              |
|          |                                |                                |
| 16       | 0.44                           | 0.56                           |

Table 8: Contingency table to assess the stationarity of the state a.

Using the table, the function performs the  $\chi^2$  test by calling the chisq.test function. This test returns a list of the chi-squared value, the degrees of freedom, and the p-value for each state. If the p-value is greater than the given significance level, we cannot reject the hypothesis that the chain is stationary.

```
R> assessStationarity(rain$rain, 10)
$`6+`
```

Pearson's Chi-squared test

```
data: mat
X-squared = 39.6145, df = 2188, p-value = 1
```

\$`1-5`

Pearson's Chi-squared test

```
data: mat
X-squared = 35.8653, df = 2188, p-value = 1
```

\$`0`

Pearson's Chi-squared test

```
data: mat
X-squared = 29.5508, df = 2188, p-value = 1
```

Divergence test for empirically estimated transition matrices

In order to test if two empirically estimated transition matrices m1 and m2 are different, we use the  $\phi$ -divergence test (Pardo 2005) that is given by

$$T_n^{\phi}(m_1, m_2, mc) = \frac{2n}{\phi''(1)} \sum_{i=1}^{M} \frac{v_{i*}}{n} \sum_{j=1}^{M} m_2(i, j) \phi\left(\frac{m_1(i, j)}{m_2(i, j)}\right)$$
(19)

where mc is the markov chain sequence, n is the length of the sequence, M is the number of states,  $v_{i*}$  is the number of transitions starting from the state i, and  $\phi$  is

$$\phi(x) = x \log x - x + 1. \tag{20}$$

The Divergence test statistic is: 0 the Chi-Square d.f. are: 2 the p-value is: 1 \$statistic

[1] 0

\$p.value
[1] 1

# 6. Applications

This section shows applications of DTMC in various fields.

## 6.1. Weather forecasting

Markov chains provide a simple model to predict the next day's weather given the current meteorological condition. The first application herewith shown is the "Land of Oz example" from J. G. Kemeny, J. L.Snell, and G. L. Thompson (1974), the second is the "Alofi Island Rainfall" from P. J. Avery and D. A. Henderson (1999).

Land of Oz

The Land of Oz is acknowledged not to have ideal weather conditions at all: the weather is snowy or rainy very often and, once more, there are never two nice days in a row. Consider three weather states: rainy, nice and snowy. Let the transition matrix be as in the following:

```
R> mcWP <- new("markovchain", states = c("rainy", "nice", "snowy"),
+ transitionMatrix = matrix(c(0.5, 0.25, 0.25,
+ 0.5, 0, 0.5,
+ 0.25,0.25,0.5), byrow = T, nrow = 3))</pre>
```

Given that today it is a nice day, the corresponding stochastic row vector is  $w_0 = (0, 1, 0)$  and the forecast after 1, 2 and 3 days are given by

```
R> W0 <- t(as.matrix(c(0, 1, 0)))
R> W1 <- W0 * mcWP; W1

    rainy nice snowy
[1,]    0.5    0    0.5

R> W2 <- W0 * (mcWP ^ 2); W2

    rainy nice snowy
[1,]    0.375    0.25    0.375

R> W3 <- W0 * (mcWP ^ 3); W3

    rainy nice snowy
[1,]    0.40625    0.1875    0.40625</pre>
```

As can be seen from  $w_1$ , if in the Land of Oz today is a nice day, tomorrow it will rain or snow with probability 1. One week later, the prediction can be computed as

[1,] 0.4000244 0.1999512 0.4000244

The steady state of the chain can be computed by means of the steadyStates method.

```
R> q <- steadyStates(mcWP)
R> q
     rainy nice snowy
[1,]     0.4     0.2     0.4
```

Note that, from the seventh day on, the predicted probabilities are substantially equal to the steady state of the chain and they don't depend from the starting point, as the following code shows.

```
R> R0 <- t(as.matrix(c(1, 0, 0)))
R> R7 <- R0 * (mcWP ^ 7); R7

rainy nice snowy
[1,] 0.4000244 0.2000122 0.3999634
```

```
R> SO <- t(as.matrix(c(0, 0, 1)))
R> S7 <- SO * (mcWP ^ 7); S7

rainy nice snowy
[1,] 0.3999634 0.2000122 0.4000244
```

## Alofi Island Rainfall

Alofi Island daily rainfall data were recorded from January 1st, 1987 until December 31st, 1989 and classified into three states: "0" (no rain), "1-5" (from non zero until 5 mm) and "6+" (more than 5mm). The corresponding dataset is provided within the **markovchain** package.

```
R> data("rain", package = "markovchain")
R> table(rain$rain)
0 1-5 6+
548 295 253
```

The underlying transition matrix is estimated as follows.

```
R> mcAlofi <- markovchainFit(data = rain$rain, name = "Alofi MC")$estimate
R> mcAlofi
```

Alofi MC

```
A 3 - dimensional discrete Markov Chain with following states 0 1-5 6+  
The transition matrix (by rows) is defined as follows 0 \qquad 1-5 \qquad 6+
```

0 1-5 6+ 0 0.6605839 0.2299270 0.1094891

1-5 0.4625850 0.3061224 0.2312925

6+ 0.1976285 0.3122530 0.4901186

The long term daily rainfall distribution is obtained by means of the steadyStates method.

R> steadyStates(mcAlofi)

```
0 1-5 6+
[1,] 0.5008871 0.2693656 0.2297473
```

## 6.2. Finance and Economics

Other relevant applications of DTMC can be found in Finance and Economics.

#### *Finance*

Credit ratings transitions have been successfully modelled with discrete time Markov chains. Some rating agencies publish transition matrices that show the empirical transition probabilities across credit ratings. The example that follows comes from **CreditMetrics** R package (Wittmann 2007), carrying Standard & Poor's published data.

It is easy to convert such matrices into markovchain objects and to perform some analyses

[1] "D"

#### *Economics*

For a recent application of **markovchain** in Economic, see Jacob (2014). A dynamic system generates two kinds of economic effects (Bard 2000):

- 1. those incurred when the system is in a specified state, and
- 2. those incurred when the system makes a transition from one state to another.

Let the monetary amount of being in a particular state be represented as a m-dimensional column vector  $c^{S}$ , while let the monetary amount of a transition be embodied in a  $C^{R}$  matrix in which each component specifies the monetary amount of going from state i to state j in a single step. Henceforth, Equation 21 represents the monetary of being in state i.

$$c_i = c_i^{S} + \sum_{j=1}^{m} C_{ij}^{R} p_{ij}.$$
 (21)

Let  $\bar{c} = [c_i]$  and let  $e_i$  be the vector valued 1 in the initial state and 0 in all other, then, if  $f_n$  is the random variable representing the economic return associated with the stochastic process at time n, Equation 22 holds:

$$E[f_n(X_n)|X_0 = i] = e_i P^n \bar{c}.$$
 (22)

The following example assumes that a telephone company models the transition probabilities between customer/non-customer status by matrix P and the cost associated to states by matrix M.

```
R> statesNames <- c("customer", "non customer")
R> P <- zeros(2); P[1, 1] <- .9; P[1, 2] <- .1; P[2, 2] <- .95; P[2, 1] <- .05;
R> rownames(P) <- statesNames; colnames(P) <- statesNames
R> mcP <- new("markovchain", transitionMatrix = P, name = "Telephone company")
R> M <- zeros(2); M[1, 1] <- -20; M[1, 2] <- -30; M[2, 1] <- -40; M[2, 2] <- 0
```

If the average revenue for existing customer is +100, the cost per state is computed as follows.

```
R> c1 <- 100 + conditionalDistribution(mcP, state = "customer") %*% M[1,] R> c2 <- 0 + conditionalDistribution(mcP, state = "non customer") %*% M[2,]
```

For an existing customer, the expected gain (loss) at the fifth year is given by the following code.

```
R> as.numeric((c(1, 0)* mcP ^ 5) %*% (as.vector(c(c1, c2))))
[1] 48.96009
```

## 6.3. Actuarial science

Markov chains are widely applied in the field of actuarial science. Two classical applications are policyholders' distribution across Bonus Malus classes in Motor Third Party Liability (MTPL) insurance (Section 6.3.1) and health insurance pricing and reserving (Section 6.3.2).

## MPTL Bonus Malus

Bonus Malus (BM) contracts grant the policyholder a discount (enworsen) as a function of the number of claims in the experience period. The discount (enworsen) is applied on a premium that already allows for known (a priori) policyholder characteristics (Denuit, Maréchal, Pitrebois, and Walhin 2007) and it usually depends on vehicle, territory, the demographic profile of the policyholder, and policy coverages deep (deductible and policy limits). Since the proposed BM level depends on the claim on the previous period, it can be modelled by a discrete Markov chain. A very simplified example follows. Assume a BM scale from 1 to 5, where 4 is the starting level. The evolution rules are shown in Equation 23:

$$bm_{t+1} = \max(1, bm_t - 1) * (\tilde{N} = 0) + \min(5, bm_t + 2 * \tilde{N}) * (\tilde{N} \ge 1).$$
 (23)

The number of claim  $\tilde{N}$  is a random variable that is assumed to be Poisson distributed.

```
+
             bmMatr[2, 1] \leftarrow dpois(x = 0, lambda)
             bmMatr[2, 4] \leftarrow dpois(x = 1, lambda)
+
             bmMatr[2, 5] \leftarrow 1 - ppois(q = 1, lambda)
             bmMatr[3, 2] \leftarrow dpois(x = 0, lambda)
             bmMatr[3, 5] \leftarrow 1 - dpois(x=0, lambda)
             bmMatr[4, 3] \leftarrow dpois(x = 0, lambda)
             bmMatr[4, 5] \leftarrow 1 - dpois(x = 0, lambda)
             bmMatr[5, 4] \leftarrow dpois(x = 0, lambda)
             bmMatr[5, 5] \leftarrow 1 - dpois(x = 0, lambda)
             stateNames <- as.character(1:5)</pre>
             out <- new("markovchain", transitionMatrix = bmMatr,
                   states = stateNames, name = "BM Matrix")
            return(out)
+
   }
R>
```

Assuming that the a-priori claim frequency per car-year is 0.05 in the class (being the class the group of policyholders that share the same common characteristics), the underlying BM transition matrix and its underlying steady state are as follows.

```
R> bmMc <- getBonusMalusMarkovChain(0.05)
R> as.numeric(steadyStates(bmMc))
```

#### [1] 0.895836079 0.045930498 0.048285405 0.005969247 0.003978772

If the underlying BM coefficients of the class are 0.5, 0.7, 0.9, 1.0, 1.25, this means that the average BM coefficient applied on the long run to the class is given by

```
R> sum(as.numeric(steadyStates(bmMc)) * c(0.5, 0.7, 0.9, 1, 1.25))
```

#### [1] 0.534469

This means that the average premium paid by policyholders in the portfolio almost halves in the long run.

## Health insurance example

Actuaries quantify the risk inherent in insurance contracts evaluating the premium of insurance contract to be sold (therefore covering future risk) and evaluating the actuarial reserves of existing portfolios (the liabilities in terms of benefits or claims payments due to policyholder arising from previously sold contracts). Key quantities of actuarial interest are: the expected present value of future benefits, PVFB, the (periodic) benefit premium, P, and the present value of future premium PVFP. A level benefit premium could be set equating at the beginning of the contract PVFB = PVFP. After the beginning of the contract the

benefit reserve is the difference between PVFB and PVFP. The example comes from Deshmukh (2012). The interest rate is 5%, benefits are payable upon death (1000) and disability (500). Premiums are payable at the beginning of period only if the policyholder is active. The contract term is three years.

The policyholders is active at  $T_0$ . Therefore the expected states at  $T_1, \ldots T_3$  are calculated in the following.

```
R> T0 <- t(as.matrix(c(1, 0, 0, 0)))
R> T1 <- T0 * mcHI
R> T2 <- T1 * mcHI
R> T3 <- T2 * mcHI
```

The present value of future benefit at T0 is given by

The yearly premium payable whether the insured is alive is as follows.

```
R > P < -PVFB / (T0[1] * 1.05 ^- 0 + T1[1] * 1.05 ^ -1 + T2[1] * 1.05 ^ -2)
```

The reserve at the beginning of the second year, in the case of the insured being alive, is as follows.

```
R> PVFB <- T2 %*% benefitVector * 1.05 ^ -1 + T3 %*% benefitVector * 1.05 ^ -2
R> PVFP <- P*(T1[1] * 1.05 ^ -0 + T2[1] * 1.05 ^ -1)
R> V <- PVFB - PVFP
R> V

[,1]
[1,] 300.2528
```

#### 6.4. Sociology

Markov chains have been actively used to model progressions and regressions between social classes. The first study was performed by Glass and Hall (1954), while a more recent application can be found in Jo Blanden and Machin (2005). The table that follows shows the income quartile of the father when the son was 16 (in 1984) and the income quartile of the son when aged 30 (in 2000) for the 1970 cohort.

## 1970 mobility

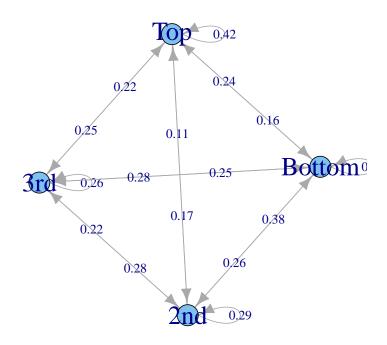


Figure 5: 1970 UK cohort mobility data.

```
R> data("blanden")
R> mobilityMc <- as(blanden, "markovchain")
R> mobilityMc
```

## Unnamed Markov chain

A 4 - dimensional discrete Markov Chain with following states Bottom 2nd 3rd Top

The transition matrix (by rows) is defined as follows

|                | 2nd       | 3rd       | Bottom    | Top       |
|----------------|-----------|-----------|-----------|-----------|
| ${\tt Bottom}$ | 0.2900000 | 0.2200000 | 0.3800000 | 0.1100000 |
| 2nd            | 0.2772277 | 0.2574257 | 0.2475248 | 0.2178218 |
| 3rd            | 0.2626263 | 0.2828283 | 0.2121212 | 0.2424242 |
| Top            | 0.1700000 | 0.2500000 | 0.1600000 | 0.4200000 |

The underlying transition graph is plotted in Figure 5.

The steady state distribution is computed as follows. Since transition across quartiles are shown, the probability function is evenly 0.25.

```
R> round(steadyStates(mobilityMc), 2)
```

```
Bottom 2nd 3rd Top [1,] 0.25 0.25 0.25 0.25
```

#### 6.5. Genetics and Medicine

This section contains two examples: the first shows the use of Markov chain models in genetics, the second shows an application of Markov chains in modelling diseases' dynamics.

#### Genetics

P. J. Avery and D. A. Henderson (1999) discusses the use of Markov chains in model Preprogucacon gene protein bases sequence. The preproglucacon dataset in markovchain contains the dataset shown in the package.

```
R> data("preproglucacon", package = "markovchain")
```

It is possible to model the transition probabilities between bases as shown in the following code.

#### Medicine

Discrete-time Markov chains are also employed to study the progression of chronic diseases. The following example is taken from B. A. Craig and A. A. Sendi (2002). Starting from six month follow-up data, the maximum likelihood estimation of the monthly transition matrix is obtained. This transition matrix aims to describe the monthly progression of CD4-cell counts of HIV infected subjects.

```
R> craigSendiMatr <- matrix(c(682, 33, 25, + 154, 64, 47, + 19, 19, 43), byrow = T, nrow = 3)
```

R> hivStates <- c("0-49", "50-74", "75-UP")

```
R> rownames(craigSendiMatr) <- hivStates</pre>
R> colnames(craigSendiMatr) <- hivStates</pre>
R> craigSendiTable <- as.table(craigSendiMatr)</pre>
R> mcM6 <- as(craigSendiTable, "markovchain")</pre>
R> mcM6@name <- "Zero-Six month CD4 cells transition"
R> mcM6
Zero-Six month CD4 cells transition
 A 3 - dimensional discrete Markov Chain with following states
 0-49 50-74 75-UP
                            (by rows) is defined as follows
 The transition matrix
            0 - 49
                       50 - 74
                                   75-UP
0-49 0.9216216 0.04459459 0.03378378
50-74 0.5811321 0.24150943 0.17735849
75-UP 0.2345679 0.23456790 0.53086420
As shown in the paper, the second passage consists in the decomposition of M_6 = V \cdot D \cdot V^{-1}
in order to obtain M_1 as M_1 = V \cdot D^{1/6} \cdot V^{-1}.
R> eig <- eigen(mcM6@transitionMatrix)</pre>
R> D <- diag(eig$values)</pre>
R> V <- eig$vectors
R> V %*% D %*% solve(V)
           [,1]
                       [,2]
                                    [,3]
[1,] 0.9216216 0.04459459 0.03378378
[2,] 0.5811321 0.24150943 0.17735849
[3,] 0.2345679 0.23456790 0.53086420
R > d <- D ^ (1/6)
R> M <- V %*% d %*% solve(V)
R> mcM1 <- new("markovchain", transitionMatrix = M, states = hivStates)</pre>
```

# 7. Discussion, issues and future plans

The **markovchain** package has been designed in order to provide easily handling of DTMC and communication with alternative packages.

Some numerical issues have been found when working with matrix algebra using R internal linear algebra kernel (the same calculations performed with MATLAB gave a more accurate result). Some temporary workarounds have been implemented. For example, the condition for row/column sums to be equal to one is valid up to fifth decimal. Similarly, when extracting the eigenvectors only the real part is taken.

Such limitations are expected to be overcome in future releases. Similarly, future versions of the package are expected to improve the code in terms of numerical accuracy and rapidity. An intitial rewriting of internal function in C++ by means of **Rcpp** package (Eddelbuettel 2013) has been started.

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