ORIGINAL ARTICLE

Some results about randomized binary Markov chains: Theory, computing and applications

J.-C. Cortés[a], A. Navarro-Quiles[a], J.-V. Romero[a] and M.-D. Roselló[a]

[a]Instituto Universitario de Matemática Multidisciplinar, Universitat Politècnica de València, Camino de Vera s/n, 46022, Valencia, Spain

ARTICLE HISTORY
Compiled February 11, 2018

ABSTRACT
This paper is addressed to give a generalization of the classical Markov methodology allowing the treatment of the entries of the transition matrix and initial condition as random variables instead of deterministic values lying in the interval $[0, 1]$. This permits the computation of the first probability density function (1-PDF) of the solution stochastic process taking advantage of the so-called Random Variable Transformation technique. From the 1-PDF relevant probabilistic information about the evolution of Markov models can be calculated including all one-dimensional statistical moments. We are also interested in determining the computation of distribution of some important quantities related to randomized Markov chains (steady state, hitting times, etc.). All theoretical results are established under general assumptions and they are illustrated by modelling the spread of a technology using real data.

KEYWORDS
Randomized binary Markov chain; random variable transformation technique; first probability density function; statistical moments; mathematical modelling

1. Introduction

A stochastic process (SP) is a mathematical representation that permits to describe how evolves a phenomenon over time in a probabilistic manner. Discrete Markov models, also referred to as Markov chains, are a fundamental class of SP where the outcome of an experiment depends only on the outcome of the previous experiment [2, 14]; this is known as Markov property. This property allows for a considerable reduction of parameters necessary to represent the evolution of a system modelled by such a process. Markov chains are very important and widely used to solve problems in a large number of domains such as operational research, computer science and distributed systems, communication networks, biology, physics, chemistry, economics, finance and social sciences, and medical decision making, for instance. They are often chosen as a suitable tools for modelling very different phenomena because Markov chains are fairly general and adaptable to many contexts [12, 14]. Moreover, excellent numerical techniques exist for computing statistics associated with them.

This contribution is addressed to give a generalization of classical Markov chains by randomizing the entries of the transition matrix and the initial conditions. To the

CONTACT M.-D Roselló. Email: drosello@imm.upv.es

best of our knowledge, this problem has not been considered in the extant literature yet, but randomizing parameters of a model is a technique used in another contexts. For example, the application of differential equations requires setting their inputs (coefficients, source term, initial and boundary conditions) using sampled data, thus containing uncertainty stemming from measurement errors. It leads to the area of random differential equations [5, 9, 10, 15]. An important key to obtain accurate results is to construct good estimations to model parameters [4, 11]. As a first step, we here will concentrate on the simplest type of Markov chains, usually referred to as binary Markov chains, which have two states.

Let $\{\mathbf{x}_n = (x_n^1, x_n^2)^\top,\ n = 0, 1, \ldots\}$ be a Markov chain, where n, denotes the cycle or period. Components x_n^1 and x_n^2 lie in the interval $]0, 1[$ and are usually interpreted as percentages or probabilities. Moreover, they satisfy $x_n^1 + x_n^2 = 1$ for every n. In a Markov chain, the state $\mathbf{x}_n$ is determined by the initial condition $\{\mathbf{x}_0 = (x_0^1, x_0^2)^\top$ and the transition matrix while its asymptotic behaviour only depends on the transition matrix. This matrix is a constant matrix whose entries represent the probabilities to change either from one state to another or to remain in the same state between to consecutive cycles. Although in practice these entries are usually assumed deterministic, in this contribution we generalize this feature by considering that the entries of the transition matrix are random variables (RVs) instead of deterministic constants. Obviously, these RVs are assumed to lie in the interval $[0, 1]$ because they must represent probabilities. In Figure 1, we show the flow diagram with the transitions between states.

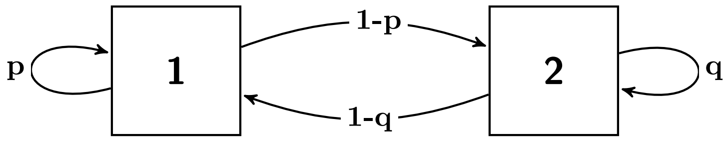

Figure 1. Flow diagram to a binary Markov chain.

In the classical context, a Markov binary chain is described as follows

$$\mathbf{x}_{n+1} = a\,\mathbf{x}_n, \quad n = 0, 1, 2, \ldots, \quad a = \begin{pmatrix} p & 1-q \\ 1-p & q \end{pmatrix}, \tag{1}$$

where a is the transition matrix and $\mathbf{x}_0 = (x_0^1, x_0^2)^\top = (x_0^1, 1 - x_0^1)^\top$ is the initial condition, i.e., the initial percentage of individuals in each group.

As indicated above, we will consider the entries of the transition matrix, p and q, as well as the initial condition, $\mathbf{x}_0$, as RVs. To distinguish RVs from deterministic variables, hereinafter RVs will be written using capital letters. So, the randomized binary Markov chain is written as

$$\begin{aligned} \mathbf{X}_{n+1} &= A\,\mathbf{X}_n, \quad n = 0, 1, 2, \ldots, \quad A = \begin{pmatrix} P & 1-Q \\ 1-P & Q \end{pmatrix}, \\ \mathbf{X}_0 &= (X_0^1, 1 - X_0^1)^\top, \end{aligned} \tag{2}$$

where X_0^1, P and Q are assumed to be absolutely continuous RVs defined on a common complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$.

A main difference with respect to classical Markov chains is that when they are randomized, apart from obtaining their solution discrete SP, $\mathbf{X}_n = (X_n^1, X_n^2)^\top =$

$(X_n^1, 1-X_n^1)^\top$, it is also important to compute its mean, $\mathbb{E}[\mathbf{X}_n]$ and its variance, $\mathbb{V}[\mathbf{X}_n]$, for each cycle n. A more general goal is the computation of its first probability density function (1-PDF), $f_1(\mathbf{x}; n)$. This function provides a full probabilistic description of the solution SP in every cycle n. From the 1-PDF, a number of statistical properties of the solution SP, such as the mean, the variance, the quartiles, confidence intervals, etc., can be straightforwardly determined. The aim of this paper is to determine the 1-PDF of the solution SP to randomized binary Markov chains under general conditions. We are also interested in determining the computation of distribution of some important quantities related to Markov chains that are very useful in practice. To reach this objective, we will apply the Random Variable Transformation (RVT) method. This is a powerful technique that has been recently used by the authors to construct random phase portrait for planar linear discrete systems [7] and to model the stroke disease [8]. This technique has been also applied in another contexts [10, 13].

This paper is organized as follows. In Section 2 some auxiliary results will be introduced. Section 3 is devoted to obtain the 1-PDF of the solution of a binary Markov chain and its stationary state. Some distributions of interesting quantities of Markov chains will be calculated in Section 4. In the last section, our findings will be applied to model the spread of a technology using real data by a binary Markov chain.

2. Preliminary results

In this section we present some results that will used throughout the paper. The RVT technique permits to compute the PDF of a RV which results from mapping of another RV whose PDF is known. The multidimensional version of the RVT technique is stated in Theorem 2.1.

Theorem 2.1. *(Multidimensional version, [15, pp. 24–25]). Let* $\mathbf{U} = (U_1, \dots, U_n)^\top$ *and* $\mathbf{V} = (V_1, \dots, V_n)^\top$ *be two* n*-dimensional absolutely continuous random vectors. Let* $\mathbf{r} : \mathbb{R}^n \to \mathbb{R}^n$ *be a one-to-one deterministic transformation of* $\mathbf{U}$ *into* $\mathbf{V}$*, i.e.,* $\mathbf{V} = \mathbf{r}(\mathbf{U})$*. Assume that* $\mathbf{r}$ *is continuous in* $\mathbf{U}$ *and has continuous partial derivatives with respect to* $\mathbf{U}$*. Then, if* $f_{\mathbf{U}}(\mathbf{u})$ *denotes the joint probability density function of vector* $\mathbf{U}$*, and* $\mathbf{s} = \mathbf{r}^{-1} = (s_1(v_1, \dots, v_n), \dots, s_n(v_1, \dots, v_n))^\top$ *represents the inverse mapping of* $\mathbf{r} = (r_1(u_1, \dots, u_n), \dots, r_n(u_1, \dots, u_n))^\top$*, the joint probability density function of vector* $\mathbf{V}$ *is given by*

$$f_{\mathbf{V}}(\mathbf{v}) = f_{\mathbf{U}}(\mathbf{s}(\mathbf{v}))\,|J|\,, \tag{3}$$

where $|J|$ *is the absolute value of the Jacobian, which is defined by*

$$J = \det\left(\frac{\partial \mathbf{s}^\top}{\partial \mathbf{v}}\right) = \det\begin{pmatrix} \dfrac{\partial s_1(v_1,\dots,v_n)}{\partial v_1} & \cdots & \dfrac{\partial s_n(v_1,\dots,v_n)}{\partial v_1} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial s_1(v_1,\dots,v_n)}{\partial v_n} & \cdots & \dfrac{\partial s_n(v_1,\dots,v_n)}{\partial v_n} \end{pmatrix}. \tag{4}$$

As the two states X_n^1 and X_n^2 of a binary Markov chain make up a closed system, $X_n^1 + X_n^2 = 1$, we shall see that once the 1-PDF of one of the two states has been computed, the 1-PDF of the other state can be straightforwardly determined taking advantage of the following key lemma.

Lemma 2.2. *Let X and Y be two absolutely continuous random variables, such as $Y = 1 - X$. Let $f_X(x)$ denote the probability density function of random variable X, then the probability density function of random variable Y is given by*

$$f_Y(y) = f_X(1-y). \tag{5}$$

This result can be derived as direct application of Theorem 2.1.

3. Solving the randomized binary Markov chain

This section is divided in two parts. In the first subsection we will compute the 1-PDF of the solution to the randomized binary Markov chain (2) under very general assumptions. The second subsection is addressed to determine the PDF of its steady state. These goals will be achieved by applying RVT technique.

In order to obtain the PDF of the solution to the randomized binary Markov chain, we need the solution of problem (2), that is given by

$$\mathbf{X}_n = A^n \mathbf{X}_0 = \begin{pmatrix} \dfrac{-1+Q+(-1+P+Q)^n\left(1-Q+(-2+P+Q)X_0^1\right)}{-2+P+Q} \\ \dfrac{-1+P+(-1+P+Q)^n\left(-1+Q-(-2+P+Q)X_0^1\right)}{-2+P+Q} \end{pmatrix}, \; n = 0, 1, \ldots \tag{6}$$

As P and Q are absolutely continuous RVs, then $\mathbb{P}\left[\{\omega \in \Omega : \, P(\omega) + Q(\omega) - 2 = 0\}\right] = 0$, for all event $\omega \in \Omega$. As a consequence, the denominator of both components of (6) is well-defined.

3.1. First Probability Density Function of $\mathbf{X}_n$

As previously indicated, in this subsection we will obtain the 1-PDF of discrete SP, $\mathbf{X}_n$, given by (6), using the RVT method. Since $\mathbf{X}_n$ is an SP and RVT method applies to RVs, first we fix the cycle n and we define the following mapping $\mathbf{r}$

$$\begin{aligned} y_1 &= r_1\left(x_0^1, p, q\right) = \frac{-1+q+(-1+p+q)^n\left(1-q+(-2+p+q)x_0^1\right)}{-2+p+q}, \\ y_2 &= r_2\left(x_0^1, p, q\right) = p, \\ y_3 &= r_3\left(x_0^1, p, q\right) = q. \end{aligned}$$

The inverse mapping $\mathbf{s}$ of $\mathbf{r}$ and its Jacobian are given by

$$\begin{aligned} x_0^1 &= s_1\left(y_1, y_2, y_3\right) = \frac{y_1\left(-2+y_2+y_3\right)+\left(-1+y_3\right)\left(-1+\left(-1+y_2+y_3\right)^n\right)}{\left(-1+y_2+y_3\right)^n\left(-2+y_2+y_3\right)}, \\ p &= s_2\left(y_1, y_2, y_3\right) = y_2, \\ q &= s_3\left(y_1, y_2, y_3\right) = y_3, \end{aligned}$$

and

$$|J| = \left|\frac{\partial s_1}{\partial y_1}\right| = \left|\frac{1}{\left(-1+y_2+y_3\right)^n}\right| \neq 0.$$

Therefore, according to Theorem 2.1 the PDF of random vector (Y_1, Y_2, Y_3), is

$$\begin{aligned} f_{y_1,y_2,y_3}(y_1,y_2,y_3) &= f_{X_0^1,P,Q}\left(\tfrac{y_1(-2+y_2+y_3)+(-1+y_3)(-1+(-1+y_2+y_3)^n)}{(-1+y_2+y_3)^n(-2+y_2+y_3)}, y_2, y_3\right) \\ &\times \left|\tfrac{1}{(-1+y_2+y_3)^n}\right|. \end{aligned}$$

Finally, marginalizing this expression with respect to P and Q and letting n arbitrary, we obtain the 1-PDF of X_n^1

$$\begin{aligned} f_1^{X^1}(x;n) &= \iint_{\mathcal{D}(P,Q)} f_{X_0^1,P,Q}\left(\tfrac{x(-2+p+q)+(-1+q)(-1+(-1+p+q)^n)}{(-1+p+q)^n(-2+p+q)}, p, q\right) \\ &\times \left|\tfrac{1}{(-1+p+q)^n}\right| \mathrm{d}q\,\mathrm{d}p, \end{aligned} \tag{7}$$

where $\mathcal{D}(P,Q)$ stands for the domain of random vector (P,Q).

Now, taking into account that $X_n^2 = 1 - X_n^1$ for every n, and applying Lemma 2.2, the 1-PDF of X_n^2 is given by

$$\begin{aligned} & f_1^{X^2}(x;n) = f_1^{X^1}(1-x;n) = \\ & = \iint_{\mathcal{D}(P,Q)} f_{x_0^1,P,Q}\left(\tfrac{(1-x)(-2+p+q)+(-1+q)(-1+(-1+p+q)^n)}{(-1+p+q)^n(-2+p+q)}, p, q\right) \left|\tfrac{1}{(-1+p+q)^n}\right| \mathrm{d}q\,\mathrm{d}p. \end{aligned} \tag{8}$$

One of the most useful applications of these explicit expressions obtained to 1-PDFs $f_1^{X^i}(x;n)$, $i = 1,2$, is the direct computation of all one-dimensional statistical moments of X_n^i,

$$\mathbb{E}\left[\left(X_n^i\right)^k\right] = \int_{\mathbb{R}} x^k f_1^{X^i}(x;n)\,\mathrm{d}x, \qquad k = 1,2,\ldots$$

Observe that if $k = 1$ one obtains the mean of X_n^i while the variance can be computed using the above moments for $k = 1,2$, since $\mathbb{V}\left[X_n^i\right] = \mathbb{E}\left[\left(X_n^i\right)^2\right] - \left(\mathbb{E}\left[X_n^i\right]\right)^2$.

3.2. First probability density function of the steady state

An important issue in dealing with Markov chains is to determine the steady state. From deterministic theory one infers the steady state to randomized Markov chain (2) is given by

$$\mathbf{X}_\infty = \begin{pmatrix} \dfrac{1-Q}{2-P-Q} \\ \dfrac{1-P}{2-P-Q} \end{pmatrix}. \tag{9}$$

Notice that $\mathbf{X}_\infty$ is well-defined because P and Q are absolutely continuous RVs, then $\mathbb{P}\left[\{\omega \in \Omega : P(\omega) + Q(\omega) - 2 = 0\}\right] = 0$, for all event $\omega \in \Omega$.

Now, we will obtain the PDF of $\mathbf{X}_\infty$. We will apply Theorem 2.1 by defining the following mapping, $\mathbf{r}$, based on expression (9)

$$\begin{array}{rcccl} y_1 & = & r_1(p,q) & = & \dfrac{1-q}{2-p-q}, \\ y_2 & = & r_2(p,q) & = & q. \end{array}$$

The inverse mapping, $\mathbf{s}$, of $\mathbf{r}$ is given by

$$\begin{array}{rcccl} p & = & s_1(y_1,y_2) & = & \dfrac{-1-y_1(-2+y_2)+y_2}{y_1}, \\ q & = & s_2(y_1,y_2) & = & y_2, \end{array}$$

and the jacobian of $\mathbf{s}$ is

$$|J| = \left|\frac{\partial s_1}{\partial y_1}\right| = \left|\frac{1-y_2}{y_1^2}\right| \neq 0.$$

Then, by applying Theorem 2.1, the PDF corresponding to the first component of the steady state, X^1_∞, is

$$f_{X^1_\infty}(x) = \int_{\mathcal{D}(Q)} f_{P,Q}\left(\frac{-1-x(2+q)+q}{x}, q\right) \left|\frac{1-q}{x^2}\right| \mathrm{d}q. \tag{10}$$

To compute the PDF corresponding to the second component of the steady state, X^2_∞, we will apply Lemma 2.2, taking into account that $X^2_\infty = 1 - X^1_\infty$, obtaining

$$\begin{array}{rcl} f_{X^2_\infty}(x) & = & f_{X^1_\infty}(1-x) = \\ & = & \displaystyle\int_{\mathcal{D}(Q)} f_{P,Q}\left(\frac{-1-(1-x)(2+q)+q}{1-x}, q\right) \left|\frac{1-q}{(1-x)^2}\right| \mathrm{d}q. \end{array} \tag{11}$$

4. Relevant probability distributions associated to randomized Markov chains

In this section the PDF of some useful quantities dealing with randomized discrete Markov chains will be obtained. These quantities are the time until a given proportion of the subpopulation is reached, the probability of first passage and the mean first passage time. In our analysis these quantities extent their deterministic counterpart to the random scenario.

4.1. Distribution of time until a given proportion of a subpopulation is reached

It is useful to know when the percentage of a group in the population will attain a certain level. This motivates the computation of the distribution of the time, N_i, $i = 1, 2$, until a given proportion, ρ_i, of the population of state i is reached. Now, we concentrate on the computation of N_1 corresponding to the first subpopulation. Then, let us consider the following relation obtained from the first component of equation (6)

$$\rho_1 = \frac{-1+q+(-1+p+q)^{n^1}(1-q+(-2+p+q)x_0^1)}{-2+p+q}. \tag{12}$$

In order to obtain the 1-PDF, $f_{N_1}(n)$, we first isolate n^1 from equation (12) and then we use the capital letter notation for random inputs X_0^1, P and Q. This yields

$$N_1 = \frac{\log\left(\frac{1-Q+(-2+P+Q)\rho_1}{1-Q+(-2+P+Q)X_0^1}\right)}{\log(-1+P+Q)}. \tag{13}$$

This RV represents the time until a percentage ρ_1 of the subpopulation 1 has been reached, so N_1 must be positive. As $\mathbb{P}\left[\{\omega\in\Omega:\, 0<P(\omega)+Q(\omega)-1<1\}\right]=1$, then $\mathbb{P}\left[\{\omega\in\Omega:\, 0<\frac{1-Q+(-2+P+Q)\rho_1}{1-Q+(-2+P+Q)X_0^1}<1\}\right]=1$ must hold in order to guarantee the positiveness of N_1. From this condition we can deduce the conditions under which N_1 can be calculated:

$$\mathbb{P}\left[\left\{\omega\in\Omega:\, X_0^1(\omega)<\rho_1<\frac{1-Q(\omega)}{2-P(\omega)-Q(\omega)}\right\}\right]=1, \tag{14}$$

or

$$\mathbb{P}\left[\left\{\omega\in\Omega:\, \frac{1-Q(\omega)}{2-P(\omega)-Q(\omega)}<\rho_1<X_0^1(\omega)\right\}\right]=1. \tag{15}$$

These conditions are very intuitive. Indeed, it is easy to check that X_n^1 given by (6) is monotone respect to n. If it is a monotonically increasing (respect. decreasing) sequence, then condition (14) (respect. (15)) applies because the proportion ρ_1 will vary in the interval $[X_0^1(\omega), X_\infty^1]$ (respect. $[X_\infty^1, X_0^1(\omega)]$) determined by the initial condition and the steady state (9).

Using the RVT technique with an appropriate mapping $\mathbf{r}$ inspired in (13),

$$\begin{aligned} y_1 &= r_1\left(x_0^1,p,q\right) = \frac{\log\left(\frac{1-q+(-2+p+q)\rho_1}{1-q+(-2+p+q)x_0^1}\right)}{\log(-1+p+q)},\\ y_2 &= r_2\left(x_0^1,p,q\right) = p,\\ y_3 &= r_3\left(x_0^1,p,q\right) = q, \end{aligned}$$

it can be proved that the 1-PDF of the time until a percentage, ρ_1, of the subpopulation 1 has been reached is given by

$$\begin{aligned} f_{N_1}(n) &= \iint_{\mathbb{R}^2} f_{X_0^1,P,Q}\left(\frac{(-1+p+q)^{-n}(1-q+(-1+q)(-1+p+q)^n+\rho_1(-2+p+q))}{-2+p+q}, p, q\right)\\ &\quad\times\left|\frac{(-1+p+q)^{-n}(-1+q-\rho_1(-2+p+q))\log(-1+p+q)}{-2+p+q}\right| \mathrm{d}p\,\mathrm{d}q. \end{aligned} \tag{16}$$

Observe that, for the sake of simplicity the domain of the integral (16) has not been specified but in practice this domain must be determined taking into account conditions (14) or (15) depending upon X_n^1 is an increasing or decreasing sequence, respectively.

In an analogous way, one can compute the 1-PDF of the time, N_2, until a given proportion, ρ_2, of subpopulation 2 is reached. This 1-PDF is given by

$$f_{N_2}(n) \quad = \quad \iint_{\mathbb{R}^2} f_{X_0^1,P,Q}\left(\frac{(-1+p+q)^{-n}(-1+p+(-1+q)(-1+p+q)^n-\rho_2(-2+p+q))}{-2+p+q}, p, q\right) \times \left|\frac{(-1+p+q)^{-n}(1-p+\rho_2(-2+p+q))\log(-1+p+q)}{-2+p+q}\right| \mathrm{d}p\, \mathrm{d}q. \tag{17}$$

4.2. Distribution of the probability of the first passage

In this subsection the 1-PDF of the probability of the first passage, $f_{i,j}^{(n)}$, is obtained. $f_{i,j}^{(n)}$ is the probability starting from i, that the first visit to state j occurs at time n, [14]. If $i = j$, $f_{i,i}^{(n)}$ is called probability of first return. In addition, from $f_{i,j}^{(n)}$, $f_{i,j}$ can be calculated, that is, the probability, starting from i, that the first visit to state j occurs in a finite time. Probabilities $f_{i,j}^{(n)}$ and $f_{i,j}$ are defined by [14]

$$f_{i,j}^{(n)} = \begin{cases} P_{i,j}, & \text{if} \quad n = 1, \\ \displaystyle\sum_{l \in S\setminus\{j\}} P_{i,l} f_{l,j}^{(n-1)}, & \text{if} \quad n \geq 2, \end{cases} \tag{18}$$

and

$$f_{i,j} = P_{i,j} + \sum_{l \in S\setminus\{j\}} P_{i,l} f_{l,j} = \sum_{n=1}^{\infty} f_{i,j}^{(n)}, \tag{19}$$

where S is the state space and $P_{i,j}$ is the probability of moving from state i to state j at the next step.

In this work, discrete Markov chains with two states are studied, and then expression (18) for each pair $(i, j) \in S \times S$ is given by

$$\begin{aligned} f_{1,1}^{(n)} &= \begin{cases} P, & \text{if} \quad n = 1, \\ (1-P)Q^{n-2}(1-Q), & \text{if} \quad n \geq 2, \end{cases} \quad f_{1,2}^{(n)} = P^{n-1}(1-P),\ n \geq 1, \\ f_{2,2}^{(n)} &= \begin{cases} Q, & \text{if} \quad n = 1, \\ (1-Q)P^{n-2}(1-P), & \text{if} \quad n \geq 2, \end{cases} \quad f_{2,1}^{(n)} = Q^{n-1}(1-Q),\ n \geq 1. \end{aligned} \tag{20}$$

With regard to the expression (19), for all pair $(i, j) \in S \times S$, $f_{i,j} = 1$. Therefore all states are recurrent and then the Markov chain is also recurrent.

Now, we will obtain the 1-PDF of each expression in (20) to each cycle n. The PDF of $f_{1,1}^{(n)}$ with $n = 1$ is the PDF of the RV P, it is

$$f_1^{f_{1,1}}(x; 1) = f_P(p).$$

In order to obtain the 1-PDF of $f_{1,1}^{(n)}$, $\forall n \geq 2$, the RVT technique will be applied.

Fixed $n \geq 2$, the following transformation, $\mathbf{r}$, is considered:

$$\begin{array}{rclcl} x & = & r_1(p,q) & = & (1-p)q^{n-2}(1-q), \\ y & = & r_2(p,q) & = & q. \end{array}$$

Then, its inverse transformation, $\mathbf{s}$, is given by

$$\begin{array}{rclcl} p & = & s_1(x,y) & = & 1+\frac{xy^{2-n}}{-1+y}, \\ q & = & s_2(x,y) & = & y, \end{array}$$

and the jacobian is $|J| = |\frac{y^{2-n}}{-1+y}|$. Therefore, applying Theorem 2.1, the PDF of the random vector (X,Y) is

$$f_{X,Y}(x,y) = f_{P,Q}\left(1+\frac{xy^{2-n}}{-1+y}, y\right)\left|\frac{y^{2-n}}{-1+y}\right|.$$

Finally, taking $n \geq 2$ arbitrary, the 1-PDF of $f_{1,1}^{(n)}$ is given by

$$f_1^{f_{1,1}}(x;n) = \int_{\mathcal{D}(Q)} f_{P,Q}\left(1+\frac{xy^{2-n}}{-1+y}, y\right)\left|\frac{y^{2-n}}{-1+y}\right| \mathrm{d}y. \tag{21}$$

Following the same argument, it is easy to check that the 1-PDF of $f_{2,2}^{(n)}$ is given by

$$f_1^{f_{2,2}}(x;n) = \begin{cases} f_Q(q), & \text{if } n=1, \\ \displaystyle\int_{\mathcal{D}(Q)} f_{P,Q}\left(y, 1+\frac{xy^{2-n}}{-1+y}\right)\left|\frac{y^{2-n}}{-1+y}\right| \mathrm{d}y, & \text{if } n \geq 2. \end{cases}$$

In the case of the 1-PDF of $f_{2,1}^{(n)}$ we can not obtain analytically the inverse mapping of the function $q^{n-1}(1-q)$ for each $n \geq 1$. So, we have to obtain the inverse numerically, using for example the Lagrange-Bürman theorem [1, 3]. To determine the 1-PDF of $f_{1,2}^{(n)}$ we proceed analogously.

4.3. Distribution of the mean first passage time

For all $i,j \in S$, it can be defined the expected hitting time of state j, starting from state i, $m_{i,j}$, using the probability of first passage. That is, as we are studying a discrete Markov chain, the expectation of the probabilities $f_{i,j}^{(n)}$ is given by

$$m_{i,j} = \sum_{n=1}^{\infty} n f_{i,j}^{(n)}.$$

As it is well-Known in the literature [14], $m_{i,j}$ can be obtained from the following linear system of equations

$$m_{i,j} = 1 + \sum_{k \in S\backslash\{j\}} P_{i,k} m_{k,j}. \tag{22}$$

Then, in our case, as we have two possibles states the different expected times are the following

$$m_{1,1} = \frac{2-P-Q}{1-Q}, \quad m_{1,2} = \frac{1}{1-P}, \\ m_{2,2} = \frac{2-P-Q}{1-P}, \quad m_{2,1} = \frac{1}{1-Q}. \tag{23}$$

We can also apply RVT technique, using appropriate mappings, in order to obtain the PDF of RVs given in (23). Below, we summarize the obtained results

- PDF of $m_{1,1}$:

$$f_{m_{1,1}}(x) = \int_{\mathcal{D}(Q)} f_{P,Q}(2 + x(-1+q) - q, q)|-1+q|\mathrm{d}q. \tag{24}$$

- PDF of $m_{1,2}$:

$$f_{m_{1,2}}(x) = f_P\left(\frac{x-1}{x}\right)\frac{1}{x^2}. \tag{25}$$

- PDF of $m_{2,1}$:

$$f_{m_{2,1}}(x) = f_Q\left(\frac{x-1}{x}\right)\frac{1}{x^2}. \tag{26}$$

- PDF of $m_{2,2}$:

$$f_{m_{2,2}}(x) = \int_{\mathcal{D}(P)} f_{P,Q}(p, 2 + p(-1+x) - x)|-1+p|\mathrm{d}p. \tag{27}$$

5. An application to model the spread of a technology

In this section an application of the previous theoretical results using real data will be shown. In this example we consider the number of mobile lines per type of contract in Spain, it is, postpaid or prepaid. We assume that this situation can be modelled by a binary Markov chain (2). For this proposal we consider data provided by 'Comisión Nacional de los Mercados y la Competencia' [6]. In Table 1, the number of mobile lines per type of contract (postpaid and prepaid) and the total of number of mobile lines during the period 2001–2015 in Spain are collected.

As there are two types of contract, postpaid and prepaid, the state space is $S = \{1, 2\}$, and we assign the value 1 to postpaid lines and 2 to prepaid lines. As it is assumed that $0 < X_n^1, X_n^2 < 1$, the first step is to transform data given in Table 1 in proportions. We denote these quantities by Y_j^k, where $k \in S$ denotes the corresponding state space and $j \in J = \{0, 1, \ldots, 14\}$, corresponds to years $2001, 2002, \ldots, 2015$, respectively.

To obtain the solution, first we need to know the distributions of inputs, so, it is necessary to choose specific probability distributions to random model parameters X_0^1, P and Q. With this aim, in a second step, data collected in Table 1 (in percentage)

Year	2001	2002	2003	2004	2005
Postpaid	10 384 261	12 657 346	15 592 659	18 555 948	21 980 367
Prepaid	19 271 468	20 872 651	21 627 180	20 066 634	20 713 465
Total	29 655 729	33 530 997	37 219 839	38 622 582	42 693 832
Year	2006	2007	2008	2009	2010
Postpaid	24 794 696	27 657 855	29 310 320	30 187 230	31 420 525
Prepaid	20 880 959	20 764 615	20 313 019	20 865 463	19 968 892
Total	45 675 855	48 422 470	49 623 339	51 052 693	51 389 417
Year	2011	2012	2013	2014	2015
Postpaid	32 220 636	32 850 295	34 409 470	36 199 911	37 618 054
Prepaid	20 369 871	17 814 804	15 749 219	14 606 340	13 449 515
Total	52 590 507	50 665 099	50 158 689	50 806 251	51 067 569

Table 1. Number of mobile lines per type of contract (postpaid and prepaid) and the total of mobile lines during the period 2001–2015 in Spain. Source CNMC [6].

are used in order to assign a reliable probabilistic distributions to random inputs, P, Q and X_0^1, which hereinafter will be assumed independent RV's.

On the one hand, as X_0^1 represents the initial proportion of people that has a postpaid mobile line, we have made the decision of assuming that X_0^1 has a Uniform distribution with parameters $0 \leq a, b \leq 1$. On the other hand, P and Q are probabilities and then they lie between 0 and 1. Therefore we consider that both have Beta distributions with parameters a_1, $a_2 > 0$ and $b_1, b_2 > 0$, respectively.

As $X_n^2 = 1 - X_n^1$, we concentrate our attention on the first component of the solution SP, X_n^1. In order to determine the positive parameters a, b, a_1, a_2, b_1 and b_2, we will minimize the mean square error between data $\{Y_j^1\}_{j\in J}$ and the expectation of the solution SP, $\{X_j^1\}_{j\in J}$, which can be obtained from the 1-PDF given in (7). All the computations have been carried out using the software Mathematica® [16]. More specifically, we have used the command `NMinimize` to calculate

$$\min_{\substack{0<a,b<1\\ a_1,a_2,b_1,b_2>0}} \sum_{j\in J} (Y_j^1 - \mathbb{E}[X_j^1(a,b,a_1,a_2,b_1,b_2)])^2. \tag{28}$$

Introducing the probability distributions

$$\begin{array}{ll} X_0^1 \equiv \mathrm{U}(a,b), & 0 \leq a < b \leq 1, \\ P \equiv \mathrm{Be}(a_1,a_2), & a_1, a_2 > 0, \\ Q \equiv \mathrm{Be}(b_1,b_2), & b_1, b_2 > 0, \end{array}$$

in (28), the following adjusted parameters are obtained

$$\begin{array}{ll} a = 0.334388, & b = 0.361633, \\ a_1 = 199.218, & a_2 = 2.01382, \\ b_1 = 444.913, & b_2 = 34.0011. \end{array}$$

Once random inputs are determined, we can calculate the 1-PDF of the solution of each state and other useful quantities as it has been described in Sections 3 and 4.

At this point, it is important to highlight that our approach permits to predict the spread of mobile lines per type of contract using both punctual predictions (mean) and probabilistic predictions (confidence intervals). This is a main difference against the classical approach where only punctual predictions are provided. This distinctive feature is possible because the randomization of probabilities of transition matrix and initial conditions. Naturally, this turns out to be a more realistic prediction since sampled data usually contain uncertainty as has been pointed out earlier.

In Figure 2, proportion of postpaid mobile lines in Spain in period 2001–2015, $\{Y_j^1\}_{j\in J}$, obtained from Table 1 is represented in blue points. The expectation of $\{X_j^1\}_{j\in J}$ is represented in a solid line. We can observe a good fit between $\{Y_j^1\}_{j\in J}$ and the expected values $\{\mathbb{E}[X_j^1]\}_{j\in J}$. Also, the 75% and 95% confidence intervals are plotted. These confidence intervals have been computed as follows. Let us fix a cycle value $\hat{n} \geq 1$ and $\alpha \in (0,1)$, and secondly determine $z_1 = z_1(\hat{n})$ and $z_2 = z_2(\hat{n})$ such that

$$\int_0^{z_1} f_1^{X^1}(x;\hat{n})\,\mathrm{d}x = \frac{z}{2} = \int_{z_2}^1 f_1^{X^1}(x;\hat{n})\,\mathrm{d}x\,.$$

Then, $(1-\alpha)\times 100\%$-confidence interval is specified by

$$1-\alpha = \mathbb{P}\left(\left\{\omega\in\Omega : X_{\hat{n}}^1(\omega)\in[z_1,z_2)]\right\}\right) = \int_{z_1}^{z_2} f_1^{X^1}(x;\hat{n})\,\mathrm{d}x\,.$$

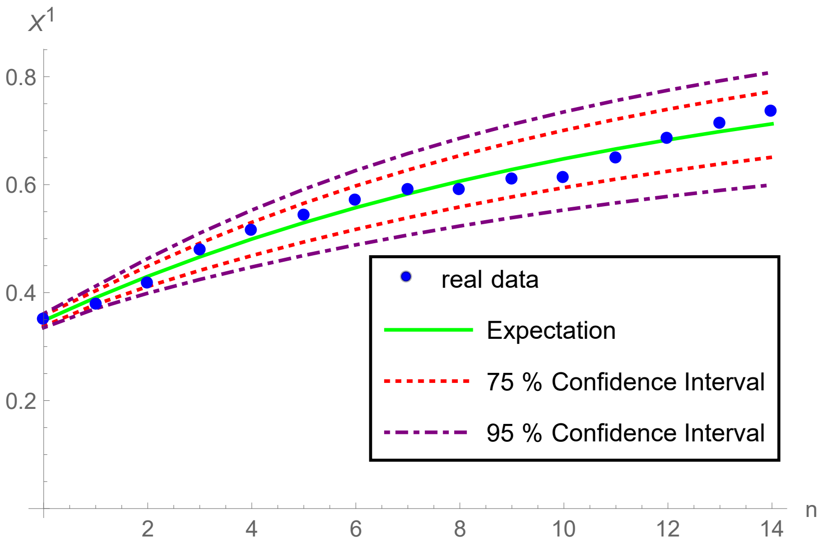

Figure 2. Expectation of postpaid mobile lines (solid line) and 75-95% confidence intervals (dotted lines). Points represent real data.

For each $n \in \mathbb{N}$ fixed, the 1-PDF of X_n^1, $f_1^{X^1}(x;n)$, is determined by (7) using the distributions of the input RVs, say, $f_{X_0^1}(x_0^1)$, $f_P(p)$ and $f_Q(q)$. As X_0^1, P and Q are assumed independent RVs, we have $f_{X_0^1,P,Q}(x_0^1,p,q) = f_{X_0^1}(x_0^1)f_P(p)f_Q(q)$. In Figure 3-left, are plotted the 1-PDF of X_n^1 at different fixed cycles: $n=1$, in blue, $n=6$ in red, $n=11$ in gray, etc. We can observe that these 1-PDFs, as $n\to\infty$, tend to the PDF of the steady state, $f_{X_\infty^1}(x)$, calculated by expression (10) and represented in black colour. Figure 3-left shows that $f_1^{X^1}(x;70)$ practically match with $f_{X_\infty^1}(x)$. The 1-PDF of X_n^2 is calculated using the transformation from $f_1^{X^1}(x;n)$ given by (8).

The analogous transformation (11) applied to $f_{X^1_\infty}(x)$ is used to determine de PDF for the steady state of X^2_n, $f_{X^2_\infty}(x)$. Results related to prepaid lines are showed in Figure 3-right. As it is expected, we can observe the symmetry of the results in both subfigures.

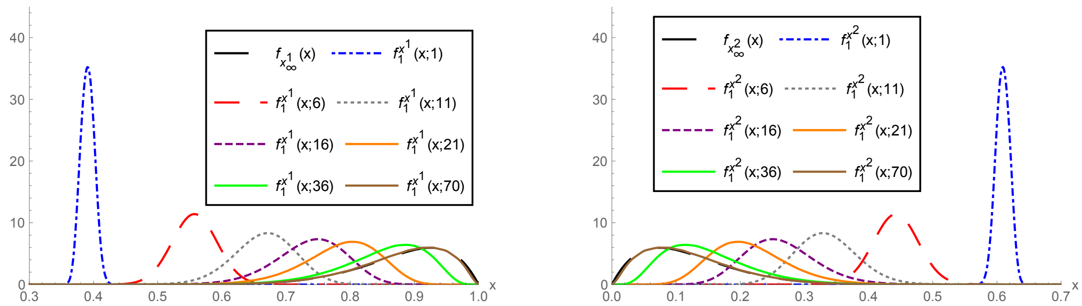

Figure 3. Left: Plot of $f_1^{X^1}(x;n)$ given by (7) for several cycles and $f_{X^1_\infty}(x)$ given by (10). Right: Plot of $f_1^{X^2}(x;n)$ given by (8) for several cycles and $f_{X^2_\infty}(x)$ given by (11).

Figure 4 shows the distribution of time until a given proportion of the population, ρ_1, possesses postpaid line mobile. This PDF is determined by equation (16) and it is represented for different values of these proportions, ρ_1. As is it expected, when the value of ρ_1 increases, the maximum of the corresponding PDFs moves to the right. In Table 2, the mean and the standard deviation of $f_{N_1}(n)$ at several values of ρ_1 are given. For example, from Figure 4, the distribution of time until a 40% of population has a postpaid mobile line reaches its maximum near 1 and it is narrow. Notice that the expectation and standard deviation in Table 2 for $\rho_1 = 0.4$ is in agreement with the representation of the corresponding PDF in Figure 4. We can observe, for each ρ_1 fixed, that PDF representations in Figure 4 are also in agreement with corresponding values of Table 2.

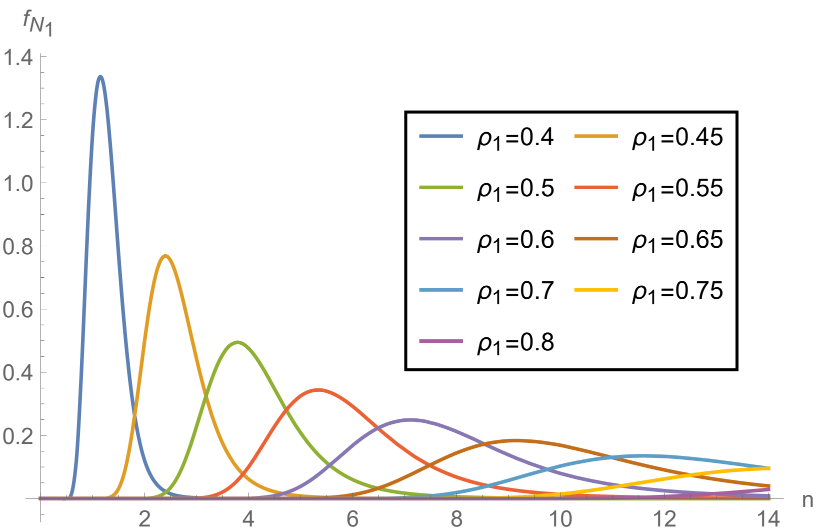

Figure 4. Plot of $f_{N_1}(n)$ given by (16) for several values of ρ_1.

ρ_1	0.4	0.45	0.5	0.55	0.6
$\mathbb{E}[f_{N_1}]$	1.275	2.648	4.207	6.0127	8.149
$\sigma[f_{N_1}]$	0.332	0.629	1.044	1.638	2.506

Table 2. Expectation and standard deviation of $f_{N_1}(n)$ (given by (16)) for several values of ρ_1.

The 1-PDF of the probability of first return $f_{1,1}^{(n)}$ given by (21) at cycle $n = 1$, it is, the probability of remaining at state 1, at cycle 1, starting from state 1 is represented in Figure 5. From representation of 1-PDF $f_1^{f_{1,1}}(x; 1)$, we can conclude that if you have a postpaid line now, you will probably have a postpaid line next year. This is in agreement with the expected value of P, $\mathbb{E}[P] = 0.98$.

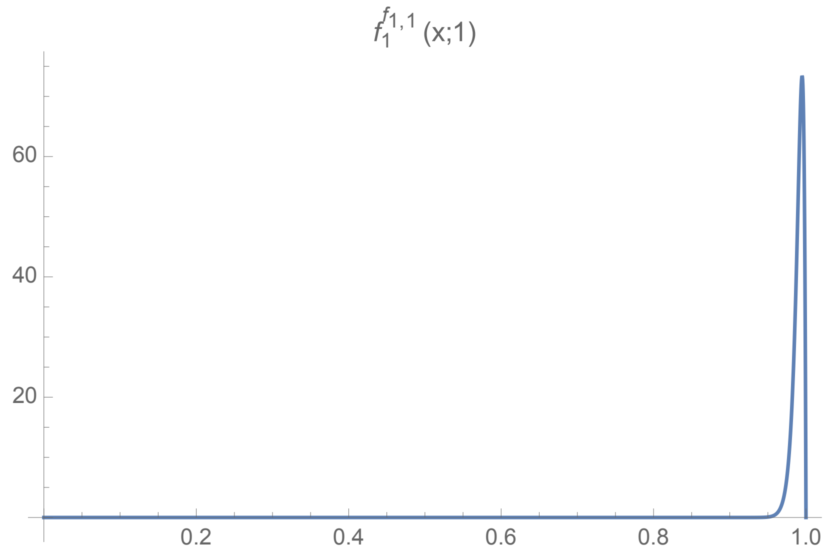

Figure 5. 1-PDF of the probability of first return $f_{1,1}^{(n)}$ given by (21) at $n = 1$.

In Figure 6-left, 1-PDF of the probability of first passage $f_{1,1}^{(n)}$ at the rest of cycles, $n \geq 2$, is plotted. The results are in agreement with Figure 5 because a little proportion of population change from postpaid line to prepaid line. In Figure 6-right the expectation plus/minus the standard deviation for $n \geq 2$ are plotted.

As it is indicated in Section 4.2, 1-PDF of first passage $f_{2,1}^{(n)}$ is calculated numerically using Lagrange-Bürman Theorem. Results for the 1-PDF of the probability of first passage $f_{2,1}^{(n)}$ are showed in the upper part of Figure 7 (top). Due to scale in vertical axis, for the sake of clarity in the presentation, it has been split in two plots. In Figure 7 (bottom), the expectation plus/minus the standard deviation for $n \geq 2$ are plotted.

Finally, in Figure 8 we show the results for the PDF of the mean first passage time between two states, $m_{i,j}$, given by (24)–(27). In Table 8 the expectation and standard deviation of each $m_{i,j}$ are provided. In both, figure and table, we observe the expected mean time passage $m_{2,1}$ is approximately 14. The expected mean time passage $m_{1,1}$ is approximately 1, in accordance with previous comments.

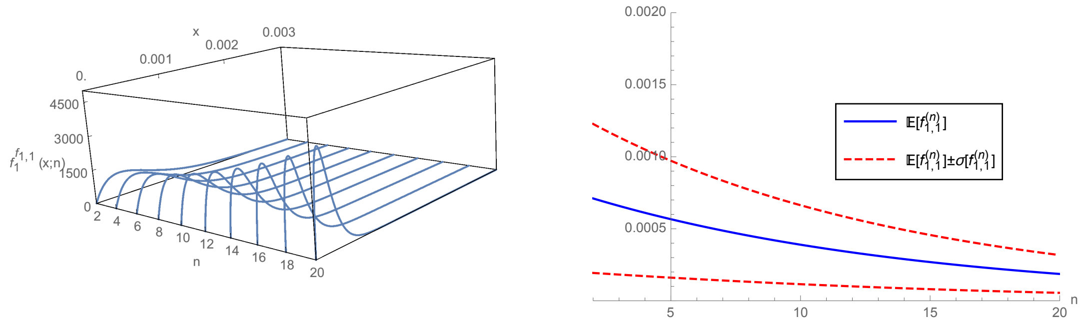

Figure 6. Left: 1-PDF of the probability of first return $f_{1,1}^{(n)}$ given by (21) at cycles $n = 2, 4, \ldots, 20$. Right: Expectation of $f_{1,1}^{(n)}$ plus/minus the standard deviation for $n \geq 2$.

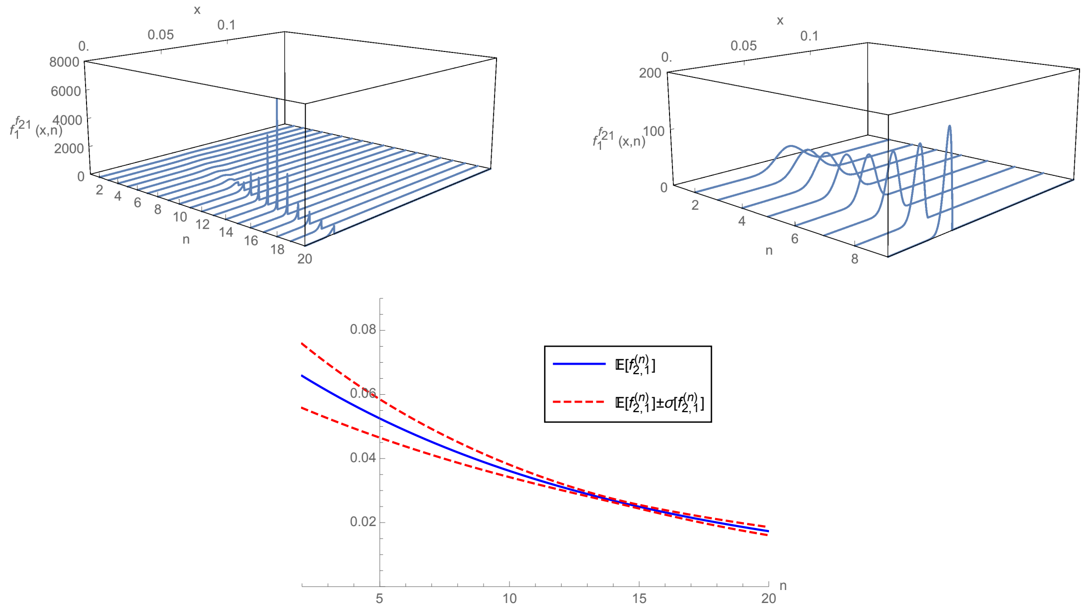

Figure 7. Top-left: 1-PDF of the probability of first return $f_{2,1}^{(n)}$ at cycles $n = 2, 3, \ldots, 20$. Top-right: Zoom of 1-PDF of the probability of first return $f_{2,1}^{(n)}$ at cycles $n = 2, 3, \ldots, 9$. Bottom: Expectation of $f_{2,1}^{(n)}$ plus/minus the standard deviation for $n \geq 2$.

	$m_{1,1}$	$m_{1,2}$	$m_{2,1}$	$m_{2,2}$
$\mathbb{E}[\cdot]$	1.14493	197.325	14.4818	14.9909
$\sigma[\cdot]$	0.105755	447.492	2.47	29.5575

Table 3. Expectation and standard deviation of the expected hitting time of state j starting from state i, $m_{i,j}$.

6. Conclusions

In this paper we have provided a full probabilistic description of the solution of a random binary Markov chain under very general assumptions on random inputs. These random inputs are the probabilities of the transition matrix and the initial condition.

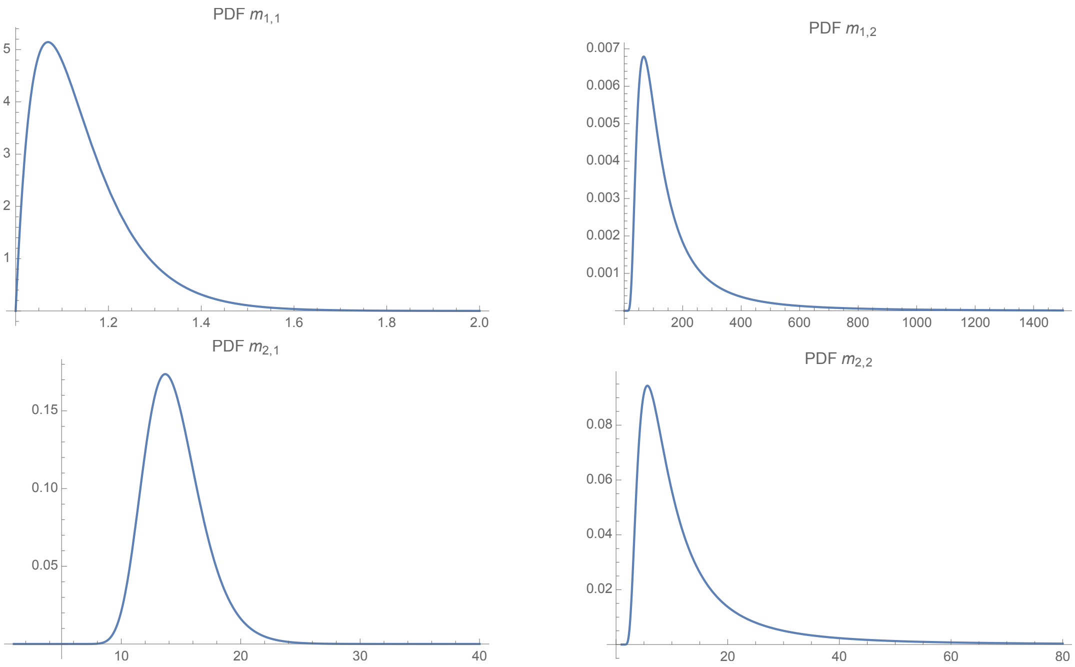

Figure 8. PDF of the expected hitting time of state j starting from state i, $m_{i,j}$, given by (24)–(27).

By means of the randomization of these probabilities, our approach provides a generalization of relevant results to classical binary Markov chains. The aforementioned full probabilistic description has been made through the first probability density function of the discrete solution stochastic process and the probability density function associated to the steady state. Furthermore, the probability density function of a key time having specific interpretation in practice has been determined. Other quantities of great interest in the deterministic context of Markov chains, like the probability of first passage time and the mean first passage time have been randomized using our approach. Then a full probabilistic description of these quantities have been established. A key mathematical tool to conduct our analysis has been the application of the Random Variable Transformation technique.

Finally we have illustrated our findings to model the percentage of mobile lines per contract type (postpaid and prepaid) in Spain using real data. This data are well-modelled through a random binary Markov chain.

Funding

This work has been partially supported by the Ministerio de Economía y Competitividad grant MTM2017-89664-P. Ana Navarro Quiles acknowledges the doctorate scholarship granted by Programa de Ayudas de Investigación y Desarrollo (PAID), Universitat Politècnica de València.

References

[1] M. Abramowitz and I.A. Stegun (eds.), *Handbook of Mathematical Functions, with Formulas, Graphs, and Mathematical Tables*, Dover, New York, 1972.

[2] E. Behrends, *Introduction to Markov Chains: With Special Emphasis on Rapid Mixing*, Advanced Lectures in Mathematics, Vieweg+Teubner Verlag, 1999.

[3] M.C. Casabán, J.C. Cortés, J.V. Romero, and M.D. Roselló, *Determining the first probability density function of linear random initial value problems by the Random Variable Transformation (RVT) technique: A comprehensive study*, Abstract and Applied Analysis 2014–ID248512 (2014), pp. 1–25.

[4] B. Chen-Charpentier and D. Stanescu, *Parameter estimation using polynomial chaos and maximum likelihood*, International Journal of Computer Mathematics 91 (2014), pp. 336–346.

[5] B. Chen-Charpentier and D. Stanescu, *Biofilm growth on medical implants with randomness*, Mathematical and Computer Modelling 54 (2011), pp. 1682–1686.

[6] CNMC, Comisión Nacional de los Mercados y la Competencia, http://data.cnmc.es/datagraph/jsp/inf_anual.jsp. Accessed: 2017-09-25.

[7] J.C. Cortés, A. Navarro-Quiles, J.V. Romero, and M.D. Roselló, *Full solution of random autonomous first-order linear systems of difference equations. application to construct random phase portrait for planar systems*, Applied Mathematics Letters 68 (2017), pp. 150–156.

[8] J.C. Cortés, A. Navarro-Quiles, J.V. Romero, and M.D. Roselló, *Randomizing the parameters of a Markov chain to model the stroke disease: A technical generalization of established computational methodologies towards improving real applications*, Journal of Computational and Applied Mathematics 324 (2017), pp. 225–240.

[9] F. Dorini, M. Cecconello, and L.B. Dorini, *On the logistic equation subject to uncertainties in the environmental carrying capacity and initial population density*, Communications in Nonlinear Science and Numerical Simulation 33 (2016), pp. 160–173.

[10] A. Hussein and M.M. Selim, *Solution of the stochastic radiative transfer equation with Rayleigh scattering using RVT technique*, Applied Mathematics and Computation 218 (2012), pp. 7193–7203.

[11] S. Kindermann and Š. Papáček, *On data space selection and data processing for parameter identification in a reaction-diffusion model based on FRAP experiments*, Abstract and Applied Analysis 2015–ID859849 (2015), pp. 1–17.

[12] J. Mar, F. Antoñanzas, R. Pradas, and A. Arrospide, *Los modelos de Markov probabilísticos en la evaluación económica de tecnologías sanitarias: una guía práctica*, Gaceta Sanitaria 24 (2010), pp. 209–214.

[13] L.T. Santos, F.A. Dorini, and M.C.C. Cunha, *The probability density function to the random linear transport equation*, Appl. Math. Comput. 216 (2010), pp. 1524–1530. Available at http://dx.doi.org/10.1016/j.amc.2010.03.001.

[14] B. Sericola, *Markov Chains: Theory, Algorithms and Applications*, Applied stochastic methods series, ISTE Ltd, London, 2013.

[15] T.T. Soong, *Random Differential Equations in Science and Engineering*, Academic Press, New York, 1973.

[16] Wolfram Research, Inc., *Mathematica* (2017). Version 11.2, Champaign, IL.