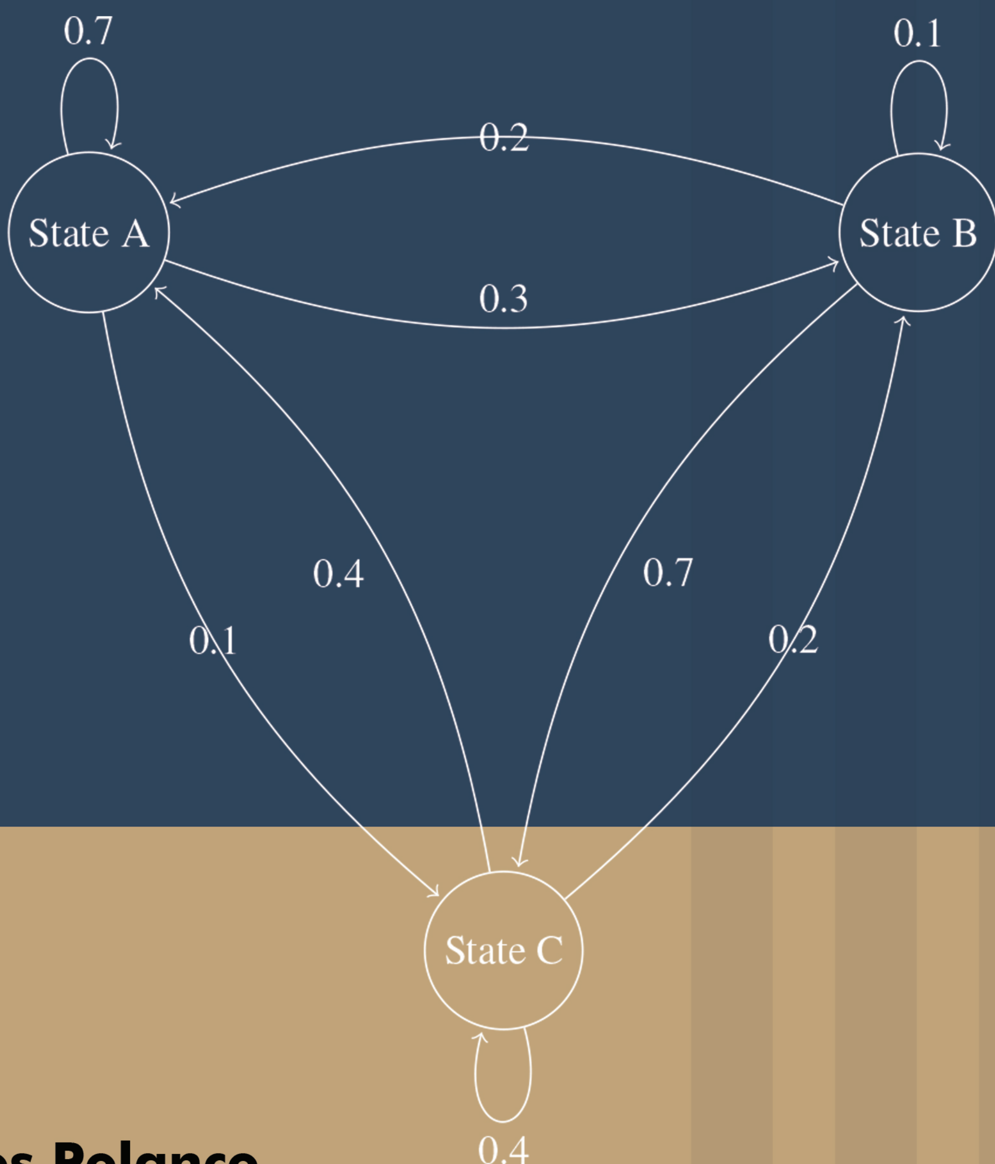
MARKOV CHAIN PROCESS

THEORY AND CASES



Carlos Polanco

Bentham Books

Markov Chain Process (Theory and Cases)

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Markov Chain Process
(Theory and Cases)

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FOREWORD I

In his book, Dr. Carlos Polanco elegantly describes fundamentals of Markov Chain Process and its applications. The author was able to overcome the usual gap between mathematicians and users, describing the main topics related to Markov Chain Process Theory in an easily apprehendable way, utilizing multiple useful examples and providing exercises. This book can be used as auxiliary book for students interested in this field as well as a reference book for seasoned Researcher.

Vladimir N. Uversky
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FOREWORD II

With Markov Chain Process, Carlos Polanco introduces an experienced view on first year in Sciences that presents a valuable reference for students as well as for their teachers. This book is very well structured, nicely written and provides a comprehensive insight into the complexity of this field. Especially, the presentation of many examples and case studies will help the readers to deepen their acquired knowledge and to relate the theory to practice. It will certainly also help researchers in related fields to refresh their knowledge and to serve as a solid and clear source on Markov Chain Process. Rounding up, Carlos Polanco's book should become part of many bookshelves.

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PREFACE

This Markov Chain Process book has been designed for students of Sciences. It contains the fundamentals related to a stochastic process that satisfies the **Markov property**. To make the comprehension of this important concept easier, all the examples, exercises, and case studies are completely solved.

In the first part, this ebook thoroughly examines the definitions of probability, independent events, mutually (and not mutually) exclusive events, conditional probability, and Bayes' theorem that are essential elements in Markov's theory.

The second part examines the Markov Chain Process elements of probability vectors, stochastic matrices, regular stochastic matrices, and fixed points. It studies the components of the matrix of transition probabilities or the transition matrix, Absorbing Markov Chain Process, and Ergodic Markov Chain Process. It also reviews two basic theorems the Law of Large Numbers and the Central Limit Theorem, under two different types of granularity discrete-time and continuous-time.

The third part of the ebook presents multiple cases in various disciplines: Predictive computational science, Urban complex systems, Computational finance, Computational biology, Complex systems theory, and Computational Science in Engineering.

The appendix section provides Fortran 90 programs and Linux scripts which allow you to reproduce the topics exposed in this work. "As of July 2022, Fortran was ranked 12th in the TIOBE programming community index, and that in addition to the C and C++ languages it is used today in scientific computing in Supercomputers platforms and High-Performance Computing clusters".

The author hopes that the reader interested in studying the fundamentals of this topic finds useful the material here presented and that the students of this field find this information motivating. The author would like to acknowledge the Faculty of Sciences at Universidad Nacional Aut´onoma de M´exico and Instituto Nacional de Cardiolog´ıa Ignacio Ch´avez for providing useful cases.

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DEDICATION

A likely impossibility is always preferable to an unconvincing possibility. The story should never be made up of improbable incidents; there should be nothing of the sort in it.

Aristotle
384 – 322 BC

List of Symbols

Symbol	**Description**	**Page**
A	Random event A	4
$P(A)$	Probability of random event A	4
Ω	Sample space	4
$P(A\|B)$	Conditional probability	4
$u_t = u_0 e^{rt}$	Malthus model	12
$u_{t+1} = Pu_t$	Leslie model	12
$u_{t+1} = Pu_t$	Lefkovitch model	15
$u_{t+1} = Pu_t$	Markov Chain Process	17
$f(t+\alpha)$	Random walks	26
P	Matrix of transition probabilities	34
P^n	Regular matrix	35
P	Absorbing matrix	36
u_0	Initial state vector	36
u_0P^n	Markov Chain Process	36
$u_f = u_0P$	Steady-state vector	62
λ_i	Eigenvalues	45
e_i	Eigenvectors	45
σ^2	Variance	53
μ	Expected value	53
$f(t,\lambda) = \lambda e^{-\lambda t}$	Exponential distribution	58
$f(k,\lambda) = \dfrac{e^{-\lambda}\lambda^k}{k!}$	Poisson distribution	59
$P^n = P$	Aperiodic matrix	62
$u_0P = 0$	Ergodicity	62
$u_f = \{u_1, u_2, \cdots, u_n\}$	Steady-state vector	63

PRELIMINARIES

The first part of the book starts with the characterization of the random functions with a review of the concepts of conditional probability and Bayes' theorem. The conditional probability is presented with over-dependent and independent random events and an extension of these concepts is introduced with the multiplication rule. Each section is self-contained so the unfamiliar reader can easily follow up on the subject.

CHAPTER 1

Probability

Abstract In this section we review the main Probability operators that are strongly associated with the main themes of this book which are Discrete-Time Markov Chain Process, and Continuous-Time Markov Chain Process. the chapter begins with the basic definition of: certain event, dependent event, independent event and impossible event. Later we review the concept of conditional probability which permeates all the following chapters as well as the multiplication rule. At the end the Bayes' Theorem is addressed which is the basis of the procedures described in the last chapters as they are: Discrete and Continuous-Time Markov Chain Process. All sections are exemplified in the simplest and most complete way possible, so that the reader does not have difficulty in the use and language of these operators in the following sections.

Keywords: Bayes' Theorem, Certain Event, Conditional Probability, Dependent Random Events, Impossible Event, Independent Random Events, Multiplication Rule, Random Event.

1.1. Introduction

Conditional probability is fundamental in Markov Chain Process as it enables the incorporation of changes that will modify the probability of random events as new information is acquired. Therefore, correct reasoning and understanding are essential in the study of statistical inference and the association of variables, particularly in the Markov Chain Process. In everyday life, sound decision-making in situations of uncertainty is largely based on conditional reasoning.

1.2. Basic Definitions

Definition 1.1. Probability P is the certainty that a **random event** occurs, it can be measured with a number between 0 and 1, where the minimum value 0 is an **impossible event** and the maximum value 1 a **certain event** [1, 2].

Example 1.1. (i) Give an example of an impossible event. (ii) Give an example of a certain event.

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Solution 1.1. (i) Number seven shown in a throw of a dice that only has the numbers 1 to 6. (ii) Any number of the dice shown in a throw.

Definition 1.2. A **random event** is a repeated experiment with an unknown result, however, we do know the possible results it could take. The set of all possible results is referred to as **sample space** Ω and a subset of the **sample space** Ω is called **random event**; it is usually defined with capital letters

The probability P of a random event is (Eq. 1.1) the repetition of a **random event** A, in relation to its sample space Ω, under controlled conditions

$$P(A) = \frac{|A|}{|\Omega|} \tag{1.1}$$

Example 1.2. Let´s take as an experiment the throwing of a dice where any of the numbers has equal probability to show. (i) Define the sample space. (ii) Define some of the random events. (iii) Define the probability of the random events defined in (ii).

Solution 1.2. (i) $\Omega = \{1,2,3,4,5\}$. (ii) $A = \{2,4,6\}$. $B = \{2,3\}$. (iii) $P(A) = \frac{3}{6}$. $P(B) = \frac{2}{6}$.

1.3. Axiomatic Construction

Definition 1.3. Let a sample space Ω where a random event $A \subset \Omega$ occurs and a real function $P : A \subset \Omega \to \mathbb{R}$ that holds:

1. For all A, $P(A) \in [0,1]$, i.e. $P : A \subset \Omega \to [0,1]$
2. If $A_1 \cap A_2 = \emptyset$ then $P(A \cup A_2) = P(A_1) + P(A_2)$
3. $P(\Omega) = 1$

1.4. Properties

- $P(\emptyset) = 0$
- For all $P(A^c) = 1 - P(A)$
- For all A_1, A_2 then $P(A \cup B) = P(A_1) + P(A_2) - P(A_1 \cap A_2)$
- If $A \cup B$, then $P(A) \leq P(B)$

1.5. Conditional Probability

Definition 1.4. Let a sample space Ω and a random event A for $P(A) > 0$ and an arbitrary random event $B \in \Omega$. The probability that a random event B occurs, as long as the random event A also occurs (in symbols $P(B|A)$), is defined as (Eq. 1.2)

$$P(B|A) = \frac{P(A \cap B)}{P(A)} \tag{1.2}$$

1.6. Random Event Types

If a sample space Ω is formed by a numerable set of n random events A_i where $A = \{A_1, A_2, \cdots, A_n\}$, then $P(A)$ is denoted as (Eq. 1.3)

$$P(A) = \sum_{i=1}^{n} P(A_i) \tag{1.3}$$

The probability of a set of random events is evaluated differently depending on whether the outcome of an event succession is affected by the outcome of the previous event or not. In this sense, there are two types of events: dependent and independent.

1.7. $P(A \cap B)$ and $P(A|B)$

The following example illustrates the difference between $P(A \cap B)$ and $P(A|B)$.

Example 1.3. Suppose 2% of a group of people has influenza and the rest is healthy. When choosing a random individual we identify that $P(sick) = 2\% = 0.02$ $P(healthy) = 98\% = 0.98$.
Let´s say that when applying a test to a healthy individual there is 3% of a false positive, i.e. $P(positive|healthy) = 3\%$ $P(negative|healthy) = 97\%$. Besides, there is a probability of 5% of false negative when testing a person for influenza, i.e. $P(negative|sick) = 5\%$ and $P(positive|sick) = 95\%$.

(i) What is the probability of finding healthy individuals that test negative? (ii) What is the probability of finding sick individuals that test positive? (iii) What is the probability to find false positives? (iv) What is the probability to find false negatives? (v) What is the probability to find positives? What is the probability that an individual is sick with influenza if the result of the test is positive?

Solution 1.3. (i) $P(healthy \cap negative) = P(healthy) \times P(negative|healthy) = 98\%$ $\times 97\% = 95.06\%$. (ii) $P(sick \cap positive) = P(sick) \times P(positive|sick) = 2\% \times 95\%$ $= 1.9\%$. (iii) $P(healthy \cap positive) = P(healthy) \times P(positive|healthy) = 98\% \times 3$ $\% = 2.94\%$. (iv) $P(sick \cap negative) = P(sick) \times P(negative|sick) = 2\% \times 5\% = 0.1$ $\%$. (v) $P(positive) = P(healthy \cap positive) + P(sick \cap positive) = 2.94\% + 1.9\% =$ 5.58%. (vi) $P(sick|positive) = \dfrac{P(sickpositive)}{P(positive)} = \dfrac{1.9\%}{5.58\%} = 34.05\%$.

1.8. Independent Random Events

Theorem 1.1. From Def. 1.2 $P(A \cap B) = P(A)P(B)$. This theorem is also known as **Multiplication Rule**.

Corollary 1.1. Let $A_1, A_2, \cdots, A_n \in \Omega$ for independent random events that comply with $P\left[\bigcap_{i=1}^{n} A_i\right] > 0$, the probability of $P\left[\bigcap_{i=1}^{n} A_i\right]$ is Eq. 1.4

CHAPTER 2

Matrix Models

Abstract This chapter describes and provides an example of the matrix models: Lefkovitch model, Leslie model, Malthus model, and stability matrix models. From these the Discrete- and Continuous-Time Markov Chain Process is introduced. These matrix models are presented as they were historically occurring, and it is highlighted how the matrix structure offers a simple algebraic solution to problems involving multiple variables, where the elements of those matrices are conditional probabilities when going from a state A (row i) to a state B (column j). Once these matrix models have been defined and exemplified, it is shown that the eigenvalues and eigenvectors of the conditional probability matrix determine the long-term stability matrix of the Markov Chain Process.

Keywords: Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Eigenvalues, Eigenvectors, Lefkovitch Model, Leslie Model, Malthus Model, Stability Matrix Models.

2.1. Introduction

This chapter describes matrix models as a practical solution to the Markov Chain Process that we will review in the following chapters. The matrix although they began as a solution to describe the long-term behavior of populations, they were soon applied to other problems. In this chapter we will show how these models can solve problems that involve multiple factors, and how the transaction between factors is solved –under matrix notation–, such as the step between elements within the matrix, where the element in row i and column j connects with the next element in that row.

It is important to note that matrix algebra involves non-laborious operations, and that as shown in this chapter it is possible to use the calculation of eigenvalues and eigenvectors of the matrix of transition probabilities to determine its long-term behavior. The calculation of these elements does not offer greater difficulty since it is a subject of Linear Algebra, although it is currently possible to determine the eigenvalues and eigenvectors through webpages.

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2.2. Malthus Model

Definition 2.1. Malthus model[3] is a process or variable that increases in size by a rate proportional to the number of elements present at each moment in time (Eq. 2.1), with this restriction, the rate of growth will always be constant so the variable will always increase in size. This model can be suitable in the short run, but it is not possible to estimate in the long run, since other variables affecting the growth are not considered in the model.

$$u_f = u_0 e^{rt} \tag{2.1}$$

Where u_t represents variable N in time t, u_0 is the size of the variable in time t_0, and r is the rate of growth of this variable.

Example 2.1. (i) Determine the population over time $t = 4$ for an initial population $u_0 = 20$ with a rate of growth of $r = 1.1$. (ii) Determine the time required to double the initial population $u_0 = 20$ with a rate of growth of $r = 1.1$.

Solution 2.1. (i) Substituting in (Eq. 2.2)

$$u_f = u_0 e^{rt} \Leftrightarrow \; u_f = 20e^{4.4} \Leftrightarrow \; u_f = 1629.02 \tag{2.2}$$

Remark 2.1. Note that in four units of time, the initial population 20 grew $\dfrac{1629}{20} \approx 81$ times.
(ii) Replacing in (Eq. 2.3) $t = 0.63$

$$2u_0 = u_0 e^{rt} \Leftrightarrow 2 = e^{1.1t} \Leftrightarrow \; \ln 2 = 1.1t \Leftrightarrow \; \frac{\ln 2}{1.1} = t \tag{2.3}$$

2.3. Leslie Model

Definition 2.2. The **Leslie model**[4] is a stratification of the **Malthus model** that separates the variable into time intervals or stages (Eq. 2.4), giving different probability values to the increasing or decreasing rates according to each stage

$$u_{t+1} = P u_t \tag{2.4}$$

u_t represents the variable u_t in time t, u_{t+1} represents the variable in time $t+1$, and matrix P represents the increase/decrease rate, where each row corresponds to a different type of variable.
Matrix P has the form (Eq. 2.5) restricted to: $a_i \geq 0, i \in \mathbb{N}$, and $0 < b_i \leq 1, i \in \mathbb{N}$

$$P = \begin{pmatrix} a_1 & a_2 & a_3 & \cdots & a_n \\ b_1 & 0 & 0 & \cdots & 0 \\ 0 & b_2 & 0 & \cdots & 0 \\ 0 & 0 & b_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & b_{n-1} & 0 \end{pmatrix} \tag{2.5}$$

Leslie matrix has this geometrical representation (Fig. 2.1).

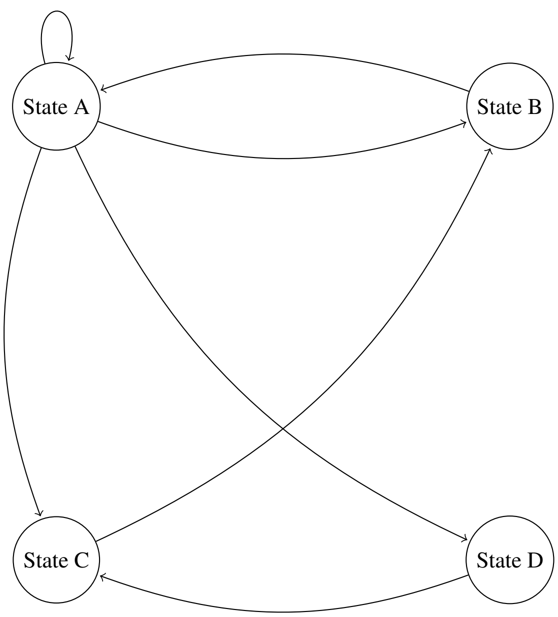

Figure 2.1: Geometrical representation of Leslie matrix.

Example 2.2. From Leslie matrix P (Eq. 2.6) and the variable in the initial time t_0 (Eq. 2.6). (i) Calculate $u_1 = Pu_0$. (ii) Calculate $u_2 = Pu_1$. (iii) Calculate $u_3 = Pu_2$. (iv) Discuss the results.

$$P = \begin{pmatrix} 0.000 & 3.000 & 1.000 & 4.000 & 2.000 \\ 0.500 & 0.0000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.2222 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.0000 & 0.444 & 0.000 & 0.000 \\ 0.000 & 0.0000 & 0.000 & 0.666 & 0.000 \end{pmatrix} \tag{2.6}$$

CHAPTER 3

Random Walks

Abstract In this chapter a review is made of the main Random walks in plane and space, and then focus on two random walks that are important to the purpose of this book: Gaussian-Dimensional Random Walk, and Markov-Dimensional Random Walk. Its definition focuses on a random process where the position at a certain moment depends only on the previous step, this particularity is called **Markov condition** and is essencially a Markov Chain Process. Random walks are used in simulation in different disciplines for their simplicity to handle phenomena involving several variables. Its use in physics, chemistry, ecology, biology, psychology and economics stands out. In this chapter we do not involve random walks in finite graphs since it is outside the purpose of this work. The definitions of these processes are accompanied by graphic and analytical examples.

Keywords: Gaussian-Dimensional Random Walk, Markov-Dimensional Random Walk, One-Dimensional Random Walk, Random Walks, Three-Dimensional Ramdom Walk, Two-Dimensional Random Walk

3.1. Introduction

A Random walk is essentially a process that allows to determine the probable location of a point, whose movement is random, and that provides the probability in each movement. Random walks are essentially a Markov processes, for which the Markov Property is met, which means that the location of a point in an instant t_i depends only on the immediate previous instant t_{i-1}. This paper describes in detail this movement in the Plane and in Space. To then focus on this type of random walks that respond to a Normal Distribution, called Gaussian-Dimensional Random Walk, and another that depends on conditional probabilities, called Markov-Dimensional Random Walk.

3.2. Random Walk

Random Walk[8] is a random process where the position of a particle at a certain moment depends on two factors, its position at a previous moment and a random

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variable that determines its direction and the length of the next step. An example of random paths is The Brownian motion.

Definition 3.1. A random walk is a function (Eq. 3.1) where $g(\alpha)$ is the random function that determines the probability of taking the next step and α is the time interval $t \in \mathbb{R}^+$ between steps.

$$f(t+\alpha) = f(t) + g(\alpha) \tag{3.1}$$

3.3. One-Dimensional Random Walk

One-Dimensional Random Walk[9] is a random walk that acts in the field of the real numbers $\mathbb{R}$. An example of this random walk is (Prog. A.1).

Example 3.1. Give an example of a one-Dimensional random walk.

Solution 3.1. Let a real line and a point (0) located at the origin. Move one unit to the right if the number shown when throwing the dice is even, or move one unit to the left if the number shown is odd. After six throws the succession would be $\{-6,-5,-3,-1,1,3,5,6\}$.

3.4. Two-Dimensional Random Walk

Two-Dimensional Random Walk[10] is a random walk that acts in the field of the real numbers $\mathbb{R}^2$. An example of this random walk is (Prog. A.2).

Example 3.2. Give an example of a two-Dimensional random walk.

Solution 3.2. Let a space in $\mathbb{R}^2$ and a point at the origin $(0,0)$. Move one unit to the right if the number shown when throwing the dice is the sum $s \in [1,3]$. Move one unit to the left if the sum is $s \in [4,6]$. Move one unit upwards if the sum is $s \in [7,9]$, and one unit downward if the sum is $s \in [10,12]$. After four double throws, the random walk will be contained in a square of 96 lattices with the centre at the origin in the space $\mathbb{R}^2$.

3.5. Three-Dimensional Random Walk

Three-Dimensional Random Walk[11] is a random walk that acts in the field of the real numbers $\mathbb{R}^3$. An example of this random walk is (Prog. A.3).

Example 3.3. Give an example of a three-Dimensional random walk.

Solution 3.3. Let a space in $\mathbb{R}^3$ and a point at the $(0,0,0)$ origin. Move one unit to the right if when throwing the dice the sum is $s \in [1,2]$. Move one unit to the left if the sum is $s \in [3,4]$. Move one unit upwards if the sum is $s \in [5,6]$. Move one unit downwards if the sum is $s \in [7,8]$. Move one unit at the front if the sum is $s \in [9,10]$. Move one unit to the back if the sum is $s \in [11,12]$. After four double throws, the random walk will be contained in a cube with 96 lattices with the centre at the origin in the space $\mathbb{R}^3$.

3.6. Gaussian-Dimensional Random Walk

Gaussian-Dimensional Random Walk[12] is a random walk that acts in the field of the real numbers $\mathbb{R}^n$ and follows a normal distribution. Example of this random walk is (Prog. A.4).

Example 3.4. Give an example of Gaussian-Dimensional Random Walk.

Solution 3.4. Let a space in $\mathbb{R}^2$ and distance d that is the result from a random number $x \in [0,2]$ in the function (Eq 3.2). Locate a point at the origin $(0,0)$ and move the length d to the right if $x \in [0,0.50]$, to the left if $x \in [0.50,1.00]$, upwards if $x \in [1.00,1.50]$, or downwards if $x \in [1.50,2.00]$

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \tag{3.2}$$

3.7. Markov-Dimensional Random Walk

Markov-Dimensional Random Walk[13] is a random walk that acts in the field of the real numbers $\mathbb{R}^n$ and follows a distribution based on the conditional probability of the states represented by the transition matrix P (Eq. 3.3).
See Chapter 5, where the Discrete-Time Markov Chain Process algorithm is described in detail

$$P = \begin{pmatrix} P(a_1|a_1) & \cdots & P(a_n|a_1) \\ P(a_1|a_2) & \cdots & P(a_n|a_2) \\ \vdots & \ddots & \vdots \\ P(a_1|a_n) & \cdots & P(a_n|a_n) \end{pmatrix} = \begin{pmatrix} p_{11} & \cdots & p_{1n} \\ p_{21} & \cdots & p_{2n} \\ \vdots & \ddots & \vdots \\ p_{n1} & \cdots & p_{nn} \end{pmatrix} \tag{3.3}$$

Example 3.5. Give an example of a Markov-Dimensional Random Walk.

Solution 3.5. A man goes daily to store A or to store B. He never goes to store A twice in a row, but if he goes to store B, then it is equally probable that he goes to store A or store B the next day. (i) Determine the matrix of transition probabilities. (ii) Draw a diagram to illustrate (i).

(i) The matrix of transition probabilities is (Eq. 3.4)

$$P = \begin{pmatrix} P(a_1|a_1) & P(a_2|a_1) \\ P(a_1|a_2) & P(a_2|a_2) \end{pmatrix} = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0.5 & 0.5 \end{pmatrix} \tag{3.4}$$

BASIC CONCEPTS

The second part of the book is dedicated to present the section Markov chain model in detail and in a practical way, and the sections Discrete-Time Markov Chain Process, Continuous-Time Markov Chain Process, and Law of Large Numbers. Each section is self-contained so the unfamiliar reader can follow up on the subject.

CHAPTER 4

Markov Chain Process

Abstract In this chapter, and from the historical introduction raised in the previous chapters, we introduce and exemplify all the components of a Markov Chain Process such as: initial state vector, Markov property (or Markov property), matrix of transition probabilities, and steady-state vector. A Markov Chain Process is formally defined and by way of categorization this process is divided into two types: Discrete-Time Markov Chain Process and Continuous-Time Markov Chain Process, which occurs as a result of observing whether the time between states in a random walk is discrete or continuous. Each of its components is exemplified, and analytically all the examples are solved.

Keywords: Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Ergodic Markov Chain Process, Initial State Vector, Markov Property, Matrix of Transition Probabilities, Regular Matrix, States, Steady-State Vector, Stochastic Matrix, Transition Probabilities

4.1. Introduction

A Markov Chain Process is a procedure that considers multiple variables evolving randomly and independently over time, when the process stabilizes it is possible to identify the development of the variables. For its characteristics, it has the potential to be used in very different fields. In this chapter we will address all its components and exemplify their use and the importance of each of them in the random process. We will address the definition of a Markov Chain Process through its definition and with an example of application so that the reader has a panoramic idea of this random process. Then we will characterize its matrix of transition probabilities as ergodic matrix from the definitions of regular matrix and absorbing matrix. Later we will define the vector of initial conditions that interacts at the beginning with the matrix of transition probabilities. Finally we will define in a general way a division to the Markov Chain Process that we will apply in the rest of the book, Discrete-Time Markov Chain Process and Continuous-Time Markov Chain Process. We will leave for the next two chapters the detailed definition and the exemplification of these last two random processes.

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4.2. Definition

A **Markov Chain Process**[14] is a succession of events where the probability that a random event occurs depends on the immediately previous event. This type of event has the particularity of "remembering" the last event, which conditions the possibilities of future events. The dependence on the previous event makes Markov Chain Process different from the succession of independent events, such as a coin tossing.

Definition 4.1. A Markov Chain Process is a process where the **transition probabilities** between **states** a_i, whose probabilities p_{ij} satisfy the **Markov property** (Eq. 4.1). That is, the probability of the state a_{i+1} only depends on the probability of the immediate preceding state a_n

$$P(a_{t+1}|a_t) \tag{4.1}$$

If t is **discrete** it is a **Discrete-Time Markov Chain Process**, on the other hand, if t is **continuous** it is a **Continuous-Time Markov Chain Process**.

4.3. Matrix of Transition Probabilities

Definition 4.2. In a Markov Chain Process, the set of probabilities p_ij between states a_i and a_j are the **conditional probabilities**[15] $P(a_j|a_i) = p_{ij}$, grouped in order in a matrix P named **Matrix of Transition probabilities** (Eq. 4.2). The sum of the rows of matrix P must always be 1

$$P = \begin{pmatrix} P(a_1|a_1) & \cdots & P(a_n|a_1) \\ P(a_1|a_2) & \cdots & P(a_n|a_2) \\ \vdots & \ddots & \vdots \\ P(a_1|a_n) & \cdots & P(a_n|a_n) \end{pmatrix} = \begin{pmatrix} p_{11} & \cdots & p_{1n} \\ p_{21} & \cdots & p_{2n} \\ \vdots & \ddots & \vdots \\ p_{n1} & \cdots & p_{nn} \end{pmatrix} \tag{4.2}$$

Example 4.1. A lady goes to store A or store B daily. She never goes to store A twice in a row, but if she goes to store B, then it is equally probable that she goes to store A or store B the next day. (i) Determine the matrix of transition probabilities. (ii) Draw a diagram to illustrate (i).

Solution 4.1. (i) The matrix of transition probabilities is (Eq. 4.3)

$$P = \begin{pmatrix} P(a_1|a_1) & P(a_2|a_1) \\ P(a_1|a_2) & P(a_2|a_2) \end{pmatrix} = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0.5 & 0.5 \end{pmatrix} \tag{4.3}$$

(ii) Here is a general diagram to illustrate this approach (Fig. 4.1)

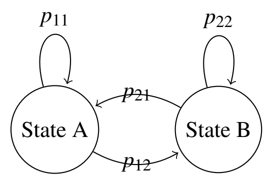

Figure 4.1: Geometrical representation of states A and B, and their conditional probabilities p_{ij}.

So, the diagram for this example is (Fig. 4.2), where the **states** A and B substitute stores A and B respectively. Let's take a closer look at the probabilities. $P(a_1|a_1) - p_{11} - 0$ is the probability that once she visited store A next day she goes there again, according to the above statement this never happens, therefore, the probability is zero. $P(a_1|a_2) = p_{21} = 0.5$ is the probability that having visited store B next day she visits store A, again the statement mentions that having visited Store B it is equally probable she visits store A or B, therefore, the probability is 0.5. Note that the order of the sub-indices p_{21} and $P(a_1|a_2)$ are reversed due to the meaning of the operators. $P(a_2|a_2) = p_{22} = 0.5$ is the probability that once she visited store B the next day she visits store B again, the statement indicates that having visited store B it is equally probably she visits store A or B, therefore, the probability is 0.5. Finally, $P(a_2|a_1) = p_{12} = 1$ is the probability that once she visited store A next day she visits store B, as the statement indicates it is not possible she visits store A twice in a row, so the probability is $p_{12} = 1$.

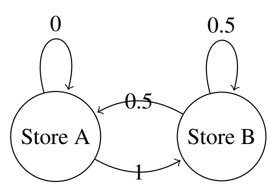

Figure 4.2: Geometrical representation of stores A and B, and their values of conditional probabilities p_{ij}.

4.4. Regular Matrix

Definition 4.3. A **regular matrix**[1] is a **matrix of transition probabilities** where all elements at the P^n power are positive.

Example 4.2. Is the matrix Ex. 4.1 regular?

Solution 4.2.

$$P^2 = \begin{pmatrix} 0 & 1 \\ 0.5 & 0.5 \end{pmatrix} \times \begin{pmatrix} 0 & 1 \\ 0.5 & 0.5 \end{pmatrix} = \begin{pmatrix} 0.5 & 0.5 \\ 0.25 & 0.75 \end{pmatrix} \tag{4.4}$$

CHAPTER 5

Discrete-Time Markov Chain Process

Abstract In this chapter, we define the Discrete-Time Markov Chain Process operator, all the initial components seen in the previous chapter are applied, and the vector of final conditions as known as steady-state vector is defined and exemplified, this vector shows the final state of the process and depends on the initial state vector and the matrix of transition probabilities. The solution mechanism is shown both by the iteration of the vector-matrix product and by determining the eigenvalues and eigenvectors of the matrix of transition probabilities. In an effort to categorize the possible matrix of transition probabilities, they are illustrated as reducible form, trasient form and recurrent form. In an effort to categorize the possible matrix of transition probabilities, they are illustrated as reducible form, trasient form and recurrent form. As a direct application of the Discrete-Time Markov process, the Metropolis Algorithm is presented, as well as a regularity that can be observed in the matrix of transition of probabilities and that is described in the section Law of Large Numbers. Some full basic examples are provided to illustrate the definition and operation of this ramdon walk.

Keywords: Discrete and Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Eigenvalues, Eigenvectors, Initial State Vector, Steady-State Vector, Markov Chain Monte Carlo, Metropolis Algorithm, Matrix of Transition Probabilities, Recurrent Form, Reducible Form, Regular Matrix, States, Steady State Vector, Stochastic Matrix, Transition Probabilities, Trasient Form.

5.1. Introduction

A **Discrete-Time Markov Chain Process** [18] is a procedure that considers multiple variables randomly evolving in a discrete-time. This can be compared to watching a movie frame by frame and not in continuous time. This section shows each component of its mechanism, as well as the calculation of the steady-state vector, as a result of the vector-matrix process and with the calculation of the invariant phase of the matrix of transition probabilities, solving its characteristic polynomial to identify the corresponding eigenvalues and eigenvectors. The algorithm of a Discrete-Time Markov Chain Process is fully exemplified and solved, and various changes are made to the model so that the dynamics of random walk can be observed. The connectivity between nodes –which is implicit in the matrix of transition probabilities–, is defined and categorized under three possible forms: irre-

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ducible, transient, and recurrent, and figures are provided that allow to understand each of these forms graphically. In its final part, this process is applied to define and solve the Metropolis algorithm as a direct application of how this type of Markov Chain Process can be used in other algorithms, and a particular type of infinite succession that can be observed in the matrix of transition of probabilities and that is described under the Law of Large Numbers.

5.2. Definition

Definition 5.1. A **Discrete-Time Markov Chain Process** is a random process where given a matrix of transition probabilities P and an initial state vector u_0, whose **states** occur in time $t \in \mathbb{N}$ that meets $u_n = u_0 P^n$, the steady-state vector u_n **only** depends on the previous vector u_{n-1}.

The **matrix of transition probabilities** P^n from step n corresponds to **time** $t = n$ and the **initial state vector** u_0 is equivalent to $u_0 P^n$.

5.3. Calculating the Stationary Distribution

The **matrix of transition probabilities**[19] P^n can be obtained by calculating the steady state vector u_f and the eigenvalues and eigenvectors e_i. This means that the matrix of transition probabilities P^n can be obtained by multiplying the matrix P by itself an n number of times, or by the two analytical methods explained below.

5.3.1. Steady-State Vector

Theorem 5.1. If the matrix of transition probabilities P is regular, then there is a **steady-state vector**[20] $u_f = (u_1, u_2, \cdots, u_n)$ that meets $u_f = u_0 P^n$, so the components of this steady-state vector u_f are the rows of the **matrix of transition probabilities** P^n.

Example 5.1. From the matrix of transition probabilities P (Eq. 5.1). (i) Determine the steady-state vector x. (ii) Determine the matrix P^n with the method in Sect. 4.7. (iii) Determine the matrix P^n using the steady-state vector. (iv) Discuss the results of (ii) and (iii). (v) Draw the corresponding diagram of the states. (vi) Determine the u_f from $u_f = u_i P^6$

$$P = \begin{pmatrix} 0.1 & 0.9 \\ 0.5 & 0.5 \end{pmatrix} \tag{5.1}$$

Solution 5.1. (i) From Eq. 5.2 we get the equations $0.1u_1 + 0.5(1 - u_1) = u$ and $0.9u_1 + 0.5(1 - u_1) = 1 - u_1$, then $u_1 = \frac{5}{14}$. The steady-state vector $u_f = (\frac{5}{14}, \frac{9}{14})$

$$(u, 1 - u) = \begin{pmatrix} 0.1 & 0.9 \\ 0.5 & 0.5 \end{pmatrix} = (u, 1 - u) \tag{5.2}$$

(ii) Multiplying matrix P (Eq. 5.2) by itself we get Eq. 5.3

$$P^6 = \begin{pmatrix} 0.35 & 0.64 \\ 0.35 & 0.64 \end{pmatrix} = \begin{pmatrix} \frac{5}{14} & \frac{9}{14} \\ \frac{5}{14} & \frac{9}{14} \end{pmatrix} \tag{5.3}$$

To illustrate these states we re-express them as follows (Eq. 5.4)

$$P = \begin{array}{c} \\ \text{State A} \\ \text{State B} \end{array} \begin{array}{c} \begin{array}{cc} \text{State A} & \text{State B} \end{array} \\ \begin{pmatrix} \frac{5}{14} & \frac{9}{14} \\ \frac{5}{14} & \frac{9}{14} \end{pmatrix} \end{array} \tag{5.4}$$

(iii) From the steady-state vector u_f the matrix of transition probabilities P^6 is (Eq. 5.5)

$$P^6 = \begin{pmatrix} \frac{5}{14} & \frac{9}{14} \\ \frac{5}{14} & \frac{9}{14} \end{pmatrix} \tag{5.5}$$

(iv) Both methods (ii) and (iii) are equivalent, however, if the squared matrix of transition probabilities P is of a large order, it is advisable to calculate the matrix power operation instead of solving the original system of equations.

(v) See Fig. 5.1

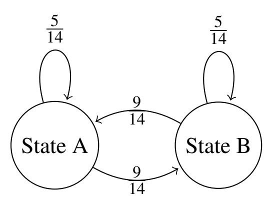

Figure 5.1: Geometrical representation of states A and B, and their values of conditional probabilities p_{ij}, taken from matrix P.

(vi) If $u_i = (u_1, u_5) = (0.5, 0.5)$ and the transition matrix P^6 (Eq. 5.5) $u_f = (0.35, 0.64)$, then in the long term, it will remain in state B with a probability of 64% and in State A with a probability of 35%

$$u_f = u_i P^6 = (0.5, 0.5) \begin{pmatrix} \frac{5}{14} & \frac{9}{14} \\ \frac{5}{14} & \frac{9}{14} \end{pmatrix} = (0.35, 0.64) \tag{5.6}$$

5.3.2. Eigenvalues and Eigenvectors

From the steady-state vector u_f Def. 6.4, where the matrix of transition probabilities P meets $u_f = uP$, we can see that the stationary distribution corresponds to the **eigenvalues**[21, 22] λ from the system $uP = \lambda u$ associated with $|P - \lambda I| = 0$ [23].

CHAPTER 6

Continuous-Time Markov Chain Process

Abstract In this chapter, we introduce through formal definitions but also with schematics and fully solved examples the main parts of the random walk Continuous-Time Markov Chain Process. This chapter is particularly oriented to the modeling of waiting lines which are cases of wide applicability in all scientific disciplines. The chapter begins by describing the Exponential and Poisson distribution which are articulated in the Continuous-Time Markov Chain Process as the elements of the matrix of conditional probabilities, and then follow the same methodology of the discrete case characterizing that matrix in aperiodic or irreducible to finally solve it as a System of Linear Equations by the usual methods or through its diagonalization by means of its eigenvalues and eigenvectors.

Keywords: Aperiodic Matrix, Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Distribution Functions, Ergodicity, Exponential Distribution, Initial State Vector, Irreducible Matrix, Markov Chain Process Markov Matrix, Poisson Distribution, Stationary Distribution, Steady-State vector, Transition Matrix Diagonalisation.

6.1. Introduction

A Continuous-Time Markov Chain Process is a model where a random variable takes positive real values in a space of S states and follows an Exponential Distribution or Poisson Distribution that meets the Markov property, showing the future behaviour of the stochastic process based on the current state. We try to approximate the solution to the continuous case in an analogous way to the discrete case so that the reader takes advantage of the entire matrix procedure, to estimate the long-term status of a random variable $T(t)$, regardless of the initial distribution. It will use a matrix of transition probabilities taking two different transition rates on a queue system.

Analogous to the discrete case we also categorize the matrix of transition probabilities in: irreducible matrix, aperiodic matrix and study the phenomenon of ergodicity that contributes to characterize a Continuous-Time Markov Chain Process. From this categorization we define the matrix of transition probabilities whose inputs are parameters of the Exponential or Paoisson Distributions, and we propose a solution as a System of Linear Equations that involves a vector-matrix operation between

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a vector of initial conditions and the matrix of transition probabilities. Its solution turns out to be the steady-state vector. Finally, we review the use of eigenvectors and eigenvalues to solve that System of Linear Equations.

Definition 6.1. A Continuous-Time Markov Chain Process is a process where the **transition probabilities** between **states** a_i whose probabilities p_{ij} satisfy the **Markov property** (Eq. 6.1). That is, the probability of the state a_{i+1} only depends on the probability of the immediate preceding state a_n.

$$P(a_{t+1}|a_t) \tag{6.1}$$

6.2. Distribution Functions

Continuous-Time Markov Chain Process is an operator that uses an Exponential Distribution (or Poisson distribution) to simulate the transition rates from state *i* to state *j*, while the inverse transition, i.e. from state *j* to state *i*, a Poisson distribution (or Exponential distribution) is used.

6.2.1. Exponential Distribution

Definition 6.2. A continuous random variable T is exponentially distributed if its function has the form Eq. 6.2 with $\lambda > 0$ and whose geometrical behaviour is Fig. 6.1.

$$f(t,\lambda) = \lambda e^{-\lambda t} \tag{6.2}$$

For $t \in \mathbb{R}^+$, where the mean of T is the reciprocal of λ, i.e. $E[T] = \dfrac{1}{\lambda}$.

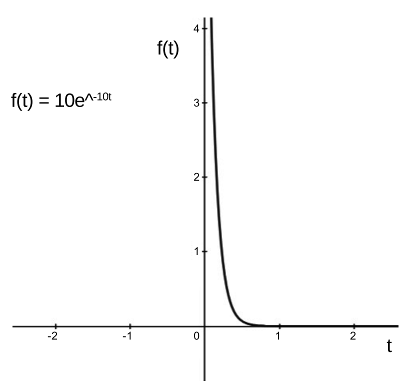

Figure 6.1: Geometrical representation of $f(t) = 10e^{-10t}$.

The Exponential Distribution meets **the Markov property**, which states that the future value of a random variable $x(t)$ only depends on its actual value and it is independent of the previous behaviour of that variable.

Proof. On one hand, the probability between 0 and t is Eq. 6.3

$$\int_0^t \lambda e^{-\lambda\alpha}\, d\alpha = 1 - e^{-\lambda t} \tag{6.3}$$

On the other hand, the probability between t_0 and $t_0 + t$ is Eq. 6.4

$$\frac{\int_{t_0}^{t_0+t} \lambda e^{-\lambda\alpha}\, d\alpha}{\int_{t_0}^{\infty} \lambda e^{-\lambda\alpha}\, d\alpha} = 1 - e^{-\lambda t} \tag{6.4}$$

Therefore, the probability does not depend on a previous event.

6.2.2. Poisson Distribution

Definition 6.3. A continuous random variable T is distributed as the Poisson distribution f if its function has the form Eq. 6.5 with $\lambda > 0$, whose geometric behaviour is Fig. 6.2

$$f(k,\lambda) = \frac{e^{-\lambda}\lambda^k}{k!} \tag{6.5}$$

For $k \in \mathbb{Z}^+$, $\lambda > 0$ represents the number of times the phenomenon is expected to occur over a time Interval t.

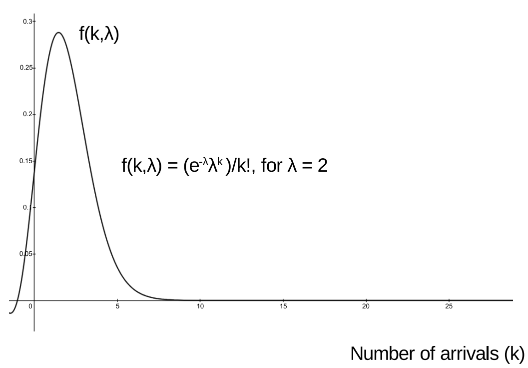

Figure 6.2: Geometrical representation of the Poisson distribution $f(k,\lambda) = \frac{e^{-\lambda}\lambda^k}{k!}$ for $\lambda = 2$.

The Poisson distribution satisfies the **Markov property** stating that the future value of a random variable $x(t)$ depends only on its present value. This can be deduced by noticing that the Poisson distribution is a variant of the Exponential distribution. Consider that $k = 1$ in Eq. 6.5 is $\frac{1}{k}\lambda e^{-\lambda}$, so the Exponential distribution characteristics are received from the Poisson distribution.

CASES

There is a wide variety of applications for the Markov Chain Process, some of them are Predictive Computational Science, Urban Complex Systems, Computational Finance, Complex Systems Theory, Computational Science in Engineering, and Computational Biology, it has also the potential for the application in new fields.

CHAPTER 7

Computational Urban Issues

Abstract This chapter defines a Discrete-Time and Continuous-Time Markov Chain Process oriented to the flow of people from one point to another in a region or city, from their transit in different neighbourhoods. This is a current problem that affects more and more countries due to the growth of communication routes and means of transport, and that has been modeled under different mathematical approaches. On the other hand, it is a multifactorial problem. In discrete type modeling we have registered in the matrix of conditional probabilities the conditional probabilities to go from a region i to another region j. In the case of continuous type modeling we have considered the rate of pedestrian mobility between regions.

Keywords: Neighbourhoods, Conditional Probabilities, Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Frequent Mobility Routes in the City, Initial State Vector, Steady-State Vector, Transition Matrix, Routes

7.1. Frequent Mobility Routes-Discrete-Time case

7.1.1. Introduction

Mobility is a multifactorial problem [34] that with new routes and means of transport is continuously transformed, it is strongly associated with population growth but involves different and varied factors such as the type of transport and the labor and recreational activity of the population. Determining the optimal route to get daily to and from a workplace in a city o region urbana, is an issue that has been addressed under very different approaches. In this section we will approximate the prediction model considering the conditional probabilities of crossing between neighborhoods. To then assume different initial positions in the region and different conditional probabilities between regions.

This can be done with a Discrete-Time Markov Chain Process, whose transition matrix P corresponds to the different sub-regions C_i that a person will use regularly to get to work (Fig. 7.1).

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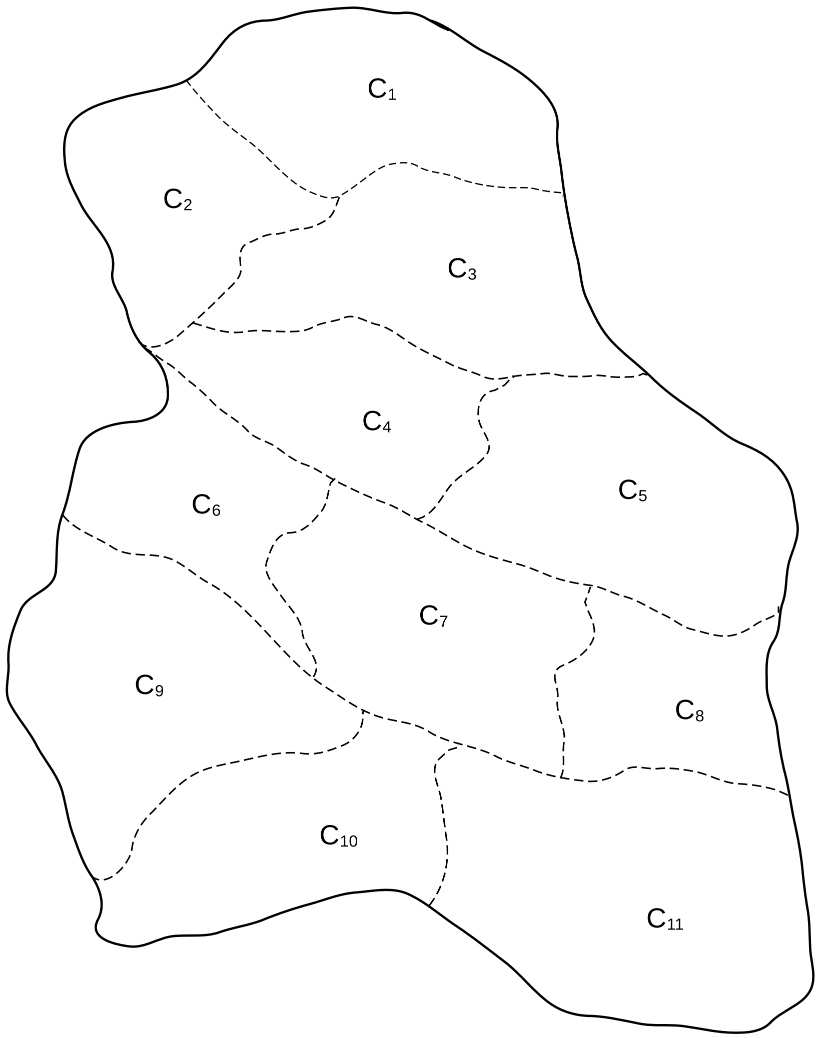

Figure 7.1: Example of a city map with the different neighbourhoods represented.

7.1.2. Materials and Methods

To design this model, 11 neighbourhoods C_i from a city were chosen (Fig. 7.1), the conditional probabilities p_{ij} represent all the routes used by the people in the neighbourhood to get to their workplace (Table 7.1). Table 7.1 expresses the relative frequencies of all the routes per inhabitant in an origin neighbourhood i when transiting to the destiny neighbourhood j.

In this sense, we are considering all possible destinations by neighbourhood and not only the representative route, as could be the farthest or nearest destination. Therefore, all the elements in each row are non-zero.

···	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}
C_1	0.09	0.09	0.09	0.08	0.10	0.10	0.10	0.08	0.09	0.09	0.09
C_2	0.09	0.09	0.09	0.09	0.09	0.10	0.10	0.09	0.08	0.09	0.09
C_3	0.09	0.09	0.09	0.07	0.11	0.10	0.10	0.09	0.08	0.09	0.09
C_4	0.09	0.09	0.09	0.07	0.12	0.09	0.10	0.08	0.09	0.08	0.10
C_5	0.09	0.10	0.10	0.07	0.10	0.09	0.10	0.08	0.09	0.09	0.09
C_6	0.10	0.09	0.09	0.08	0.08	0.09	0.11	0.09	0.09	0.09	0.09
C_7	0.08	0.08	0.09	0.09	0.10	0.12	0.10	0.06	0.08	0.10	0.10
C_8	0.10	0.10	0.08	0.11	0.09	0.13	0.10	0.07	0.08	0.10	0.10
C_9	0.10	0.09	0.07	0.11	0.09	0.13	0.08	0.06	0.06	0.09	0.11
C_{10}	0.09	0.09	0.08	0.10	0.10	0.12	0.09	0.07	0.07	0.10	0.09
C_{11}	0.11	0.08	0.07	0.09	0.10	0.08	0.10	0.10	0.09	0.09	0.09

Table 7.1: Conditional probabilities for the origin-neighbourhood (rows) and destiny-neighbourhood (columns).

The conditional probabilities in Table 7.1 were randomly built. From this table we built matrix P (Eq. 7.1).

$$P = \begin{array}{c} \\ C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \\ C_{10} \\ C_{11} \end{array} \begin{array}{c} \begin{array}{ccccccccccc} C_1 & C_2 & C_3 & C_4 & C_5 & C_6 & C_7 & C_8 & C_9 & C_{10} & C_{11} \end{array} \\ \begin{pmatrix} 0.09 & 0.09 & 0.09 & 0.08 & 0.10 & 0.10 & 0.10 & 0.08 & 0.09 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.09 & 0.09 & 0.09 & 0.10 & 0.10 & 0.09 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.09 & 0.07 & 0.11 & 0.10 & 0.10 & 0.09 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.09 & 0.07 & 0.12 & 0.09 & 0.10 & 0.08 & 0.09 & 0.08 & 0.10 \\ 0.09 & 0.10 & 0.10 & 0.07 & 0.10 & 0.09 & 0.10 & 0.08 & 0.09 & 0.09 & 0.09 \\ 0.10 & 0.09 & 0.09 & 0.08 & 0.08 & 0.09 & 0.11 & 0.09 & 0.09 & 0.09 & 0.09 \\ 0.08 & 0.08 & 0.09 & 0.09 & 0.10 & 0.12 & 0.10 & 0.06 & 0.08 & 0.10 & 0.10 \\ 0.10 & 0.10 & 0.08 & 0.11 & 0.09 & 0.13 & 0.10 & 0.07 & 0.08 & 0.10 & 0.10 \\ 0.10 & 0.09 & 0.07 & 0.11 & 0.09 & 0.13 & 0.08 & 0.06 & 0.06 & 0.09 & 0.11 \\ 0.09 & 0.09 & 0.08 & 0.10 & 0.10 & 0.12 & 0.09 & 0.07 & 0.07 & 0.10 & 0.09 \\ 0.11 & 0.08 & 0.07 & 0.09 & 0.10 & 0.08 & 0.10 & 0.10 & 0.09 & 0.09 & 0.09 \end{pmatrix} \end{array} \tag{7.1}$$

We multiply matrix P (Eq. 7.1) by itself to get matrix P^n (Eq. 7.9).

Note 7.1. For this calculations see Prog. A.10.

$$P^n = \begin{array}{c} \\ C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \\ C_{10} \\ C_{11} \end{array} \begin{array}{c} \begin{array}{ccccccccccc} C_1 & C_2 & C_3 & C_4 & C_5 & C_6 & C_7 & C_8 & C_9 & C_{10} & C_{11} \end{array} \\ \begin{pmatrix} 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.08 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.0r87 & 0.08 & 0.09 & 0.09 \\ 0.09 & 0.09 & 0.08 & 0.09 & 0.10 & 0.10 & 0.10 & 0.0r87 & 0.08 & 0.09 & 0.09 \end{pmatrix} \end{array} \tag{7.2}$$

CHAPTER 8

Computational Biology Issues

Abstract This chapter defines Discrete and Continuous-Time Markov Chain Process aimed to identify the preponderant function of a protein from the analysis of its sequence, adapting the matrix of transition probabilities so that the elements of the latter are occupied by the relative frequencies of the interactions of the pairs of amino acids located there. The chapter illustrates in detail this methodology and robustness to rescue the preponderant activity among other possible functions that the protein could offer, if minimal changes were made in its primary structure. The present approach is presumed to be used for the construction of synthetic proteins.

This chapter defines Discrete and Continuous-Time Markov Chain Process aimed to identify proteins from the specific regularities found in their sequences.

Keywords: Amino acids, Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Initial State Vector, NP Non-polar, N Polar, P^- Negative Charge, P^+ Positive Charge, Polarity Profile, Preponderant Function of Proteins, Proteins, Sequences, Steady-State Vector, Structural Proteomics, Transition Matrix

8.1. Protein Structure - Discrete-Time Case

8.1.1. Introduction

Proteins are the functional units of living organisms, they transform into tissue, organs, and bones. All the elements that make up a living organism are formed by them and so are bacteria and viruses. Proteins usually have different functions, however, some of these functions are preponderant. This last objective is a current topic for various research groups since the construction of new drugs or antibiotics that can be used to alert or strengthen the immune system of humans depends on it.

The identification of proteins from the regularities found in their sequences (linear representation of the amino acids) provides different mathematical-computational approaches, one of them is to get a polarity profile [35, 36, 37, 38, 39, 40, 41, 42] from the sequence of the protein, which is formed by amino acids that can be extracted from a group of 20.

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As every amino acid has a specific polarity profile, it can be verified if the occurrence of polarity characterizes the different functional groups of proteins. In this work, a Discrete-Time Markov Chain Process is developed whose transition matrix P represents the four different polarity groups: P^+ positive charge, P^- negative charge, N polar, and NP non-polar.

8.1.2. Materials and Methods

To build the model we considered these four polarity groups, and the conditional probabilities p_{ij} that represent the polarity groups found in a chosen set of sequences (Table 8.1). Table 8.1 expresses the relative frequency of a pair of amino acids transiting from the left amino acid i to the right amino acid j.

The procedure is to get a set of sequences representative of the characteristic sought, then we read these proteins by pairs from right to left, e.g. if the protein -expressed in the correspondent polarity values- is [P^-, N, P^+, $\cdots$], then in matrix P we add 1 in [P^-, N], and in [N, P^+], and so forth.

Assume the incidences expressed as conditional probabilities are in (Table 8.1).

$\cdots$	P^+	P^-	N	NP
P^+	0.25	0.35	0.20	0.20
P^-	0.10	0.60	0.25	0.05
N	0.05	0.15	0.70	0.10
NP	0.40	0.50	0.05	0.05

Table 8.1: Conditional probabilities for origin-polarity (rows) and final-polaridad (columns).

The conditional probabilities in Table 8.1 were randomly built. With this information we build matrix P Eq. 8.1

$$P = \begin{array}{c} \\ P^+ \\ P^- \\ N \\ NP \end{array} \begin{array}{c} \begin{array}{cccc} P^+ & P^- & N & NP \end{array} \\ \begin{pmatrix} 0.25 & 0.35 & 0.20 & 0.20 \\ 0.10 & 0.60 & 0.25 & 0.05 \\ 0.05 & 0.15 & 0.70 & 0.10 \\ 0.40 & 0.50 & 0.05 & 0.05 \end{pmatrix} \end{array} \tag{8.1}$$

Then, we multiply matrix P Eq. 8.1 by itself to get matrix P^n Eq. 8.9

Note 8.1. For this calculation see Prog. A.11.

$$P^n = \begin{array}{c} \\ P^+ \\ P^- \\ N \\ NP \end{array} \begin{array}{c} \begin{array}{cccc} P^+ & P^- & N & NP \end{array} \\ \begin{pmatrix} 0.13 & 0.38 & 0.41 & 0.09 \\ 0.13 & 0.38 & 0.41 & 0.09 \\ 0.12 & 0.37 & 0.41 & 0.09 \\ 0.13 & 0.37 & 0.41 & 0.09 \end{pmatrix} \end{array} \tag{8.2}$$

The steady-state vector $u_f = u_0 \lim_{n\to\infty} P^n$ and taking matrix P^n (Eq. 8.9) and the initial state vector $u_0 = (0.25, \cdots, 0.25)$ we get the steady-state vector u_f.

8.1.3. Results

So, if we take the initial state vector $u_0 = (1/4, \cdots, 1/4)$, we get the steady-state vector u_f (Eq. 8.3).

$$u_f = (0.125, 0.375, 0.411, 0.089) \tag{8.3}$$

When comparing u_0 (Eq. 8.4) with u_f (Eq. 8.3) we can see that the preferential polarity interactions are P^-, N, P^+, and NP.

$$u_0 = (0.250, 0.250, 0.250, 0.250) \tag{8.4}$$

However, if we change the value of the initial state vector, see u_0 (Eq. 8.5), reducing the frequency of the two polarities P^+ and P^- the steady-state vector u_f (Eq. 8.6) will show an increase at both ends of the vector u_f.

$$u_0 = (0.200, 0.200, 0.300, 0.300) \tag{8.5}$$

$$u_f = (0.125, 0.375, 0.411, 0.089) \tag{8.6}$$

Also, if we alter the values of the initial state vector u_0 (Eq. 8.7), reducing the frequency of the polarity groups N and NP, the steady-state vector u_f (Eq. 8.8) shows an increase in the central polarity groups P^- and N of the vector u_f.

$$u_0 = (0.300, 0.300, 0.200, 0.200) \tag{8.7}$$

$$u_f = (0.125, 0.375, 0.411, 0.089) \tag{8.8}$$

Finally, if we change matrix P isolating the polarity group P^+ (Eq. 8.9), we will see a significant change in the steady-state vector u_f (Eq. 8.10).

$$P = \begin{array}{c} \\ P^+ \\ P^- \\ N \\ NP \end{array} \begin{array}{c} \begin{array}{cccc} P^+ & P^- & N & NP \end{array} \\ \begin{pmatrix} 0.00 & 0.37 & 0.41 & 0.09 \\ 0.12 & 0.37 & 0.41 & 0.09 \\ 0.12 & 0.37 & 0.41 & 0.09 \\ 0.00 & 0.37 & 0.41 & 0.09 \end{pmatrix} \end{array} \tag{8.9}$$

$$u_f = (0.014, 0.082, 0.098, 0.019) \tag{8.10}$$

8.1.4. Discussion

When the elements of matrix P are modified they can provide information about the polarity group of a specific set of sequences, or produce synthetic proteins.

CHAPTER 9

Computational Financial Issues

Abstract This chapter defines Discrete or Continuous-Time Markov Chain Process aimed at predicting market trends, taking the ratings that the stock exchange gives to shares. The chapter is developed through two cases that affect in different ways the corresponding matrix of transition probabilities, in the discrete case conditional probabilities are assumed for each of the groups of shares that were registered in that matrix, and in the continuous case different forward and backward speeds between shares are assumed.

Keywords: A, AA, AAA, B, BB, BBB, C, CC, CCC, Conditional Probabilities, Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Initial State Vector, Market Trends, Stock Markets, Steady-State Vector, Transition Matrix.

9.1. Prediction of Market Trends-Discrete-Time case

9.1.1. Instroduction

Predicting the near future of the stocks from their supply and demand is a fundamental issue in financial markets [43]. Here, we develop a Discrete-Time Markov Chain Process whose matrix of transition probabilities P represents the the probability of moving from one share to another among these possibilities AAA, AA, A, BBB, BB, B, CCC, CC, C, D. A share depends on the supply and demand and these are susceptible to multiple factors of a different kind. Knowing the progression of a share or block of shares in the medium term is crucial for financial decision-makers. In this work, we develop a Discrete-Time Markov Chain Process whose matrix of transition probabilities P corresponds to the ten described types of ratings that a share can have, with AAA being the highest value share, and D the lowest value share.

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9.1.2. Materials and Methods

To build the model ten types of shares will be taken and the conditional probabilities p_{ij} will represent the rating groups found in the block of shares (Table 9.1). Table 9.1 expresses the relative frequencies of the shares when moving from one type of share i to the next j.

The procedure is to select a block of shares to build all possible conditioned probabilities, considering that in ten types of ratings there will be 81 different transitions.

Assume that the incidences are expressed as conditional probabilities (Table 9.1).

···	*AAA*	*AA*	*A*	*BBB*	*BB*	*B*	*CCC*	*CC*	*C*	*D*
AAA	0.90	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
AA	0.40	0.50	0.03	0.01	0.01	0.01	0.01	0.01	0.01	0.01
A	0.01	0.40	0.50	0.03	0.01	0.01	0.01	0.01	0.01	0.01
BBB	0.01	0.01	0.40	0.50	0.03	0.01	0.01	0.01	0.01	0.01
BB	0.01	0.01	0.01	0.40	0.50	0.03	0.01	0.01	0.01	0.01
B	0.01	0.01	0.01	0.01	0.40	0.50	0.03	0.01	0.01	0.01
CCC	0.01	0.01	0.01	0.01	0.01	0.40	0.50	0.03	0.01	0.01
CC	0.01	0.01	0.01	0.01	0.01	0.01	0.40	0.50	0.03	0.01
C	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.40	0.50	0.03
D	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.03	0.40	0.50

Table 9.1: Conditional probabilities for initial-shares (rows) and final-shares (columns).

The conditional probabilities in Table 9.1 were built at random and matrix P (Eq. 9.1) was built with this information.

$$P = \begin{array}{c} \\ AAA \\ AA \\ A \\ BBB \\ BB \\ B \\ CCC \\ CC \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cccccccccc} AAA & AA & A & BBB & BB & B & CCC & CC & C & D \end{array} \\ \begin{pmatrix} 0.90 & 0.02 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.40 & 0.50 & 0.03 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.40 & 0.50 & 0.03 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.40 & 0.50 & 0.03 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.40 & 0.50 & 0.03 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.40 & 0.50 & 0.03 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.40 & 0.50 & 0.03 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.40 & 0.50 & 0.03 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.40 & 0.50 & 0.03 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.03 & 0.40 & 0.50 \end{pmatrix} \end{array} \tag{9.1}$$

Then, we multiply matrix P Eq. 9.1 by itself to get matrix P^n Eq. 9.9.

Note 9.1. See this calculation Prog. A.12.

$$P^n = \begin{array}{c} \\ AAA \\ AA \\ A \\ BBB \\ BB \\ B \\ CCC \\ CC \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cccccccccc} AAA & AA & A & BBB & BB & B & CCC & CC & C & D \end{array} \\ \begin{pmatrix} 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \\ 0.42 & 0.09 & 0.08 & 0.08 & 0.07 & 0.07 & 0.06 & 0.05 & 0.03 & 0.02 \end{pmatrix} \end{array} \quad (9.2)$$

Taking the steady-state vector $u_f = u_0 \lim_{n\to\infty} P^n$, matrix P^n (Eq. 9.9) and the initial state vector $u_0 = (0.10, \cdots, 0.10)$ we get the steady-state vector u_f.

9.1.3. Results

If we take the initial state vector $u_0 = (1/10, \cdots, 1/10)$ we get the steady-state vector u_f Eq. 9.3

$$u_f = (0.421, 0.093, 0.085, 0.081, 0.076, 0.070, 0.062, 0.052, 0.038, 0.021) \quad (9.3)$$

When comparing u_0 (Eq. 9.4) with u_f (Eq. 9.3) we find that the preferred type of share is AAA.

$$u_0 = (0.100, 0.100, 0.100, 0.100, 0.100, 0.100, 0.100, 0.1000.100, 0.100) \quad (9.4)$$

However, if we change the values of the initial state vector, see u_0 Eq. 9.5, reducing the frequency of the AAA and AA shares, the steady-state vector u_f (Eq. 9.6) shows a substantial decrement in the AAA u_f shares.

$$u_0 = (0.050, 0.050, 0.050, 0.250, 0.100, 0.100, 0.100, 0.1000.100, 0.100) \quad (9.5)$$

$$u_f = (0.421, 0.093, 0.085, 0.081, 0.076, 0.070, 0.062, 0.052, 0.038, 0.021) \quad (9.6)$$

And if we change the values of the initial state vector u_0 Eq. 9.7, reducing the frequency of the CC, C and D shares, the steady-state vector u_f (Eq. 9.8) does not show a substantial change compared to vector u_f (Eq. 9.6).

$$u_0 = (0.010, 0.100, 0.100, 0.100, 0.100, 0.100, 0.100, 0.2500.050, 0.000) \quad (9.7)$$

$$u_f = (0.421, 0.093, 0.085, 0.081, 0.076, 0.070, 0.062, 0.052, 0.038, 0.021) \quad (9.8)$$

CHAPTER 10

Computational Science Issues

Abstract This chapter introduces a Hierarchical Markov Chain Process over a hierarchical network whose nodes are Discrete-Time Markov Chain and Continuous-Time Markov Chain Processes. We consider it useful to carry out this non-exhaustive analysis to discuss the advantages and disadvantages of a random walk of this nature and its possible application, particularly in real-time and in unsupervised mode. Examples are provided under the discrete and continuous schemes.

Keywords: Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Hierarchical Markov Process, Homogeneous Markov Chain Process, Initial State Vector, Steady-State Vector, Transition Matrix

10.1. Hierarchical Markov Chain Process - Discrete-Time Case

10.1.1. Introduction

This chapter introduces the Hierarchical Markov Chain Process (HMCP), over a hierarchical network whose elements or nodes are Discrete-Time Markov Chain Processes. The structure of an HMCP is a directed network where the different states are determined within various Discrete-Time Markov Chain Processes (Fig. 10.1), so the steady-state vector of a process i is the initial state vector of a process j. This chapter is not intended to be exhaustive, but to exemplify how it is possible to couple Discrete-Time Markov Chain Processes in a network, providing this network with random walks. This introduction is accompanied by a numerical example and it explains how to modify the network.

In this sense, a Hierarchical Markov Chain Process is a Semi-Markov Process or Markov renewal process.

Note 10.1. "Semi-Markovian processes provide a very flexible structure for modelling phenomena that evolve over time as they combine the probabilistic structure of a Markov chain and a renewal process. In other words, semi-Markovian processes model systems whose transitions between states occur according to a

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Markov chain and the times at which such transitions occur are random and form a process of renewal” [44].

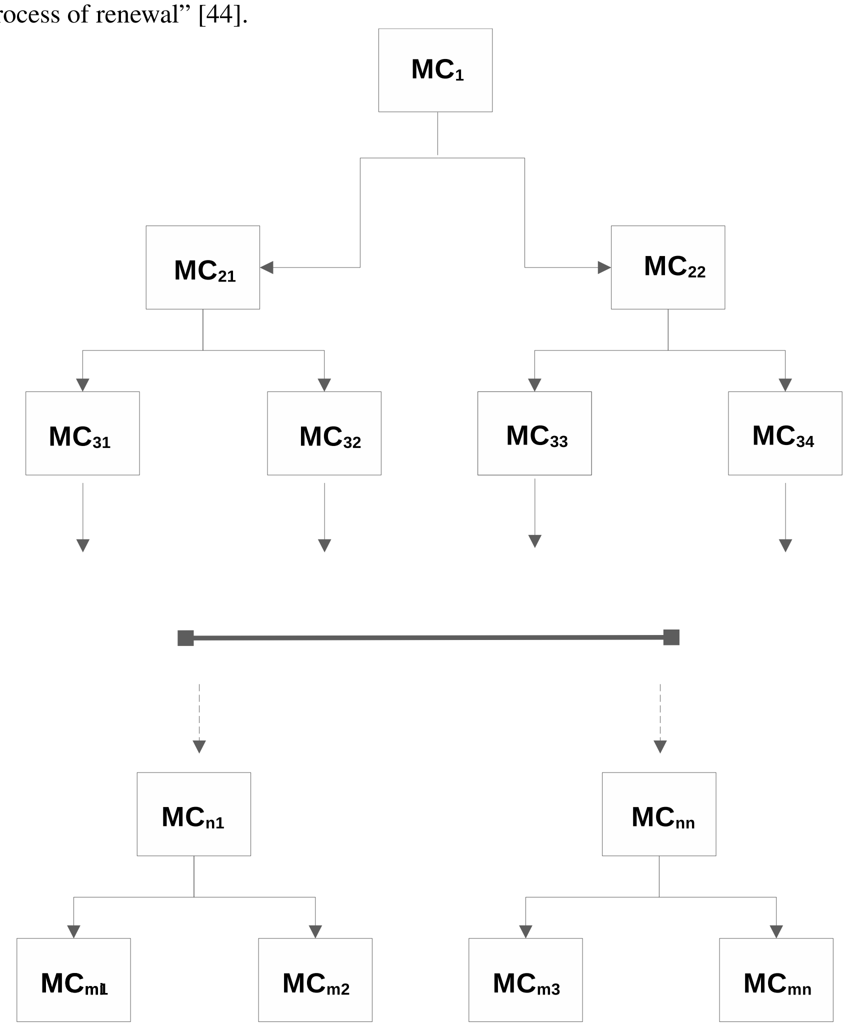

Figure 10.1: Example of the structure of a Hierarchical Markov Chain Process.

Schematically, the process presented here fractally replicates an MC over the entire region, in multiple MC_{ij} over each subregion resulting from partitioning the original region, so each MC_{ij} will be representative of that subregion.

If we coloured each subregion of the value of the steady-state vector u_f, we could see continuity between the two adjacent subregions.

10.1.2. Materials and Methods

To build the model, we have n levels and each level has m Discrete-Time Markov Chain Processes (MC_{ij}) (Fig. 10.1). The conditional probabilities p_{ij} represent all the states (Table 10.1). Table 10.1 expresses the relative frequencies of the states when transiting from one to another i.e., from the initial-state i to the final-state j.

In this sense, all possible states in MC_{ij} are considered, therefore, all the elements in each row are non-zero.

···	A	B	C	D
A	p_{11}	p_{12}	p_{13}	p_{14}
B	p_{21}	p_{22}	p_{23}	p_{24}
C	p_{31}	p_{32}	p_{33}	p_{34}
D	p_{41}	p_{42}	p_{43}	p_{44}

Table 10.1: Conditional probabilities p_{ij} of MC_{ij}.

10.1.3. Results

The conditional probabilities in Table 10.1 were randomly built. This information was used for the matrix of transition probabilities P (Eq. 10.1). Note that each MC_{ij} has a matrix P and all these matrices must have the same dimension.

$$P = \begin{array}{c} \\ A \\ B \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{pmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{21} & p_{22} & p_{23} & p_{24} \\ p_{31} & p_{32} & p_{33} & p_{34} \\ p_{41} & p_{42} & p_{43} & p_{44} \end{pmatrix} \end{array} \tag{10.1}$$

Then, we multiply matrix P_{ij} (Eq. 10.1) by itself to get matrix P_{ij}^n (Eq. 10.2).

$$P_{ij}^n = \begin{array}{c} \\ A \\ B \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{pmatrix} q_{11} & q_{12} & q_{13} & q_{14} \\ q_{21} & q_{22} & q_{23} & q_{24} \\ q_{31} & q_{32} & q_{33} & q_{34} \\ q_{41} & q_{42} & q_{43} & q_{44} \end{pmatrix} \end{array} \tag{10.2}$$

Since the steady-state vector $u_{ij}^f = u_{ij}^0 \lim_{n\to\infty} P_{ij}^n$, where matrix P_{ij}^n is matrix P multiplied n times by itself (Eq. 10.2), the initial state vector u_{ij}^0 is the vector that feeds the process MC_{ij}, and the steady-state vector u_{ij}^f is the resultant vector of the process MC_{ij}.

For convenience, if there is no hierarchy in the Hierarchical Markov Chain Process, it will be called Homogeneous Markov Chain Process, particularly if it is used to develop an application to know the dissemination of an epidemic outbreak [45].

CHAPTER 11

Computational Medicine Issues

Abstract This chapter first introduces a Discrete-Time Markov Chain Process aimed to predict the spread of a disease in a region, based on the census of the subjects: **S**, susceptible; **Ia**, Active infected; **In**, Inactive infected; **Na** Subject dead by natural causes; **Nm** Subject killed by the disease. Later, is introduced a Continuous-Time Markov Chain Process to predict the spread of a disease based on different census of the subjects: **S**, number of susceptible individuals; **I**, number of infected individuals; and **R** number of recovery individuals. Both methods are known to be effective in issuing early warnings for serious respiratory infections. Both cases are exemplified and discussed.

Keywords: Conditional Probabilities, Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Epidemic Disease, Hierarchical Markov Chain Process, Homogeneous Markov Chain Process, Initial State Vector, Markov Chain Process, Steady-State Vector, Transition Matrix

11.1. Pandemic Spread Rate-Discrete-Time Case

11.1.1. Instroduction

The spread of a disease with pandemic potential is a public security issue, whose impact claims millions of human lives and impacts all countries. An early warning allows to reduce the number of infections and consequently deaths, on the other hand, however there is no general criterion to decree such an alert. This work aims to determine the future changes of five states associated with the process described: **S**, susceptible; **Ac**, Active infected; **In**, Inactive infected; **Na** Subject dead by natural causes; **Nm** Subject killed by the disease [46, 47, 48].

The profile of these five states characterize with a fingerprint a disease with pandemic potential. This work develops a Discrete-Time Markov Chain Process whose transition matrix of transition probabilities *P* corresponds to these five states.

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11.1.2. Materials and Methods

To construct the model, these five states are taken and the conditional probabilities p_{ij} represent the figures found in a region (Table 11.1). Table 11.1 expresses the relative frequencies to transit from state i to state j.

Assume that the incidences expressed as conditional probabilities are in Table 11.1.

$\cdots$	S	Ia	In	Na	Nm
S	0.15	0.25	0.20	0.20	0.20
Ac	0.10	0.35	0.45	0.05	0.05
In	0.05	0.15	0.30	0.40	0.10
Na	0.00	0.00	0.00	0.85	0.15
Nm	0.00	0.00	0.00	0.15	0.85

Table 11.1: Conditional probabilities for an initial-disease (rows) and final-disease (columns).

The conditional probabilities of Table 11.1 were built at random and they were used for matrix P Eq. 11.1

$$P = \begin{array}{c} \\ S \\ Ac \\ In \\ Na \\ Nm \end{array} \begin{array}{c} \begin{array}{ccccc} S & Ia & In & Na & Nm \end{array} \\ \begin{pmatrix} 0.15 & 0.25 & 0.20 & 0.20 & 0.20 \\ 0.10 & 0.35 & 0.45 & 0.05 & 0.05 \\ 0.05 & 0.15 & 0.30 & 0.40 & 0.10 \\ 0.00 & 0.00 & 0.00 & 0.85 & 0.15 \\ 0.00 & 0.00 & 0.00 & 0.15 & 0.85 \end{pmatrix} \end{array} \tag{11.1}$$

Then, matrix P Eq. 11.1 was multiplied by itself to get matrix P^n (Eq. 11.9).

Note 11.1. For this calculation see Prog. A.13.

$$P^n = \begin{array}{c} \\ S \\ Ac \\ In \\ Na \\ Nm \end{array} \begin{array}{c} \begin{array}{ccccc} S & Ia & In & Na & Nm \end{array} \\ \begin{pmatrix} 0.00 & 0.00 & 0.00 & 0.50 & 0.50 \\ 0.00 & 0.00 & 0.00 & 0.50 & 0.50 \\ 0.00 & 0.00 & 0.00 & 0.50 & 0.50 \\ 0.00 & 0.00 & 0.00 & 0.50 & 0.50 \\ 0.00 & 0.00 & 0.00 & 0.50 & 0.50 \end{pmatrix} \end{array} \tag{11.2}$$

Since the steady-state vector $u_f = u_i \lim_{n\to\infty} P^n$, taking matrix P^n (Eq. 11.9) and the initial state vector $u_0 = (0.25, \cdots, 0.20)$, we get the steady-state vector u_f.

11.1.3. Results

Taking the initial state vector $u_0 = (1/5, \cdots, 1/5)$, we get the steady-state vector u_f Eq. 11.3

$$u_f = (0.000, 0.000, 0.500, 0.500) \tag{11.3}$$

When comparing u_0 (Eq. 11.4) with u_f (Eq. 11.3) we can see that the most chosen states are Na y Nm.

$$u_0 = (0.200, 0.200, 0.200, 0.200) \tag{11.4}$$

However, if we change the values of the initial state vector, see u_0 (Eq. 11.5), reducing the frequency of the two first states S and Ac, the steady-state vector u_f (Eq. 11.6) shows an accumulation at the ends of the vector u_f (Fig. 7.1).

$$u_0 = (0.100, 0.100, 0.260, 0.260, 0.260) \tag{11.5}$$

$$u_f = (0.000, 0.000, 0.001, 0.493, 0.486) \tag{11.6}$$

And if we change the values of the initial state vector u_0 (Eq. 11.7), reducing the frequency of the states Na and Nm, the steady-state vector u_f (Eq. 11.8) shows the same distribution of vector u_f (Eq. 11.6).

$$u_0 = (0.260, 0.260, 0.260, 0.100, 0.100) \tag{11.7}$$

$$u_f = (0.000, 0.001, 0.001, 0.494, 0.483) \tag{11.8}$$

Finally, if we change matrix P decreasing the state S (Eq. 11.9), we will not see a significant modification in the steady-state vector u_f (Eq. 11.10).

$$P = \begin{array}{c} \\ S \\ Ac \\ In \\ Na \\ Nm \end{array} \begin{array}{c} \begin{array}{ccccc} S & Ia & In & Na & Nm \end{array} \\ \begin{pmatrix} 0.00 & 0.40 & 0.20 & 0.20 & 0.20 \\ 0.00 & 0.35 & 0.45 & 0.05 & 0.05 \\ 0.00 & 0.15 & 0.30 & 0.40 & 0.10 \\ 0.00 & 0.00 & 0.00 & 0.85 & 0.15 \\ 0.00 & 0.00 & 0.00 & 0.15 & 0.85 \end{pmatrix} \end{array} \tag{11.9}$$

$$u_f = (0.000, 0.000, 0.000, 0.500, 0.500) \tag{11.10}$$

11.1.4. Discussion

If the elements of the transition matrix P are modified, they can provide information about the pandemic potential of a region to feature this region or to compare it with other regions.

The Discrete-Time Markov Chain Process approach to determine the spread of a disease from the variables **S**, Susceptible subject; **Ac**, Active infected; **In**, Inactive infected; **Na** Subject dead of natural causes; and **Nm** Subject killed by the disease, is an extension of other approaches.

One of these approaches uses three variables **S**, Susceptible subject; **I**, Infected subject; and **R** Recovered subject, which provides a simple and powerful model to predict a close future from the stabilization of the Markov Chain Process.

CHAPTER 12

Computational Social Sciences Issues

Abstract This chapter defines a Discrete-Time and Continuous-Time Markov Chain Process aimed to identify the language used to write a text. This is a brief introduction to show the usefulness of both random walks in the recognition of a language, and how these methods can lead to deepen the recognition using other possible structural language. An example is established and solved from diphthongs of the English language.

Keywords: Conditional Probabilities, Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Discrete-Time and Continuous-Time Markov Chain Process, English Diphthongs, Initial State Vector, Matrix of Transition Probabilities, Natural Language Recognition, Steady-State Vector, Transition Matrix.

12.1. Natural Language Recognition - Discrete-Time Case

12.1.1. Instroduction

The identification of the language in which a text is written from the frequency of its consonants and vowels [49] is a topic that has been approached in different ways. In this work, we developed a Discrete-Time Markov Chain Process whose matrix of transition probabilities P uses English diphthongs. The elements of the matrix correspond to the frequency of the diphthongs in the text, so the matrix represents the profile of the language of the text and the Discrete-Time Markov Chain Process uses it to identify the same language in other texts.

12.1.2. Materials and Methods

The following text was used to build this model:

—"The noise was ended now. The smoke drifted like thin, gray wisps of fog above the tortured earth and the shattered fences and the peach trees that had been whittled

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into toothpicks by the cannon fire. For a moment silence, if not peace, fell upon those few square miles of ground where just a while before men had screamed and torn at one another in the frenzy of old hate and had contended in an ancient striving and then had fallen apart, exhausted."— [Clifford Simak, "Way Station",1963].

The conditional probabilities p_{ij} represent the occurrence of the English diphthongs found in the text {ay, ea, ee, ie, oi, oo, and ow} (Table 12.1). Table 12.1 expresses the absolute frequency of the occurrences of all these diphthongs when reading the text from left to right

It should be noted that a typical Discrete-Time Markov Chain Process would have considered the occurrences when reading the text, however, this work addresses this issue in a more restrictive way since the diphthongs are in English language and, therefore, some occurrences will be zeros (Table 12.1).

···	a	e	i	o	u	w	y
a	0.00	0.00	0.00	0.00	0.00	0.00	1.00
e	4.00	1.00	0.00	0.00	0.00	0.00	0.00
i	0.00	1.00	0.00	0.00	0.00	0.00	0.00
o	0.00	0.00	1.00	1.00	0.00	1.00	0.00
u	0.00	0.00	0.00	0.00	0.00	0.00	0.00
w	0.00	0.00	0.00	0.00	0.00	0.00	0.00
y	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 12.1: Absolute frequencies for English diphthongs.

The conditional probabilities in (Table 12.1) were randomly built and this table was used for matrix *P* (Eq. 12.1).

$$P = \begin{array}{c} \\ a \\ e \\ i \\ o \\ u \\ w \\ y \end{array} \begin{array}{c} \begin{array}{ccccccc} a & e & i & o & w & u & w \quad y \end{array} \\ \begin{pmatrix} 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 1.000 \\ 0.800 & 0.200 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.333 & 0.333 & 0.000 & 0.333 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \end{pmatrix} \end{array} \tag{12.1}$$

Then, matrix *P* (Eq. 12.1) is multiplied by itself to get matrix P^n (Eq. 12.2).

Note 12.1. This calculation can be seen in (Prog. A.15).

$$P^n = \begin{array}{c} \\ a \\ e \\ i \\ o \\ u \\ w \\ y \end{array} \begin{array}{c} \begin{array}{ccccccc} a & e & i & o & w & u & w \quad y \end{array} \\ \begin{pmatrix} 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 1.000 \\ 0.032 & 0.008 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.014 & 0.035 & 0.035 & 0.035 & 0.000 & 0.035 & 0.033 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \end{pmatrix} \end{array} \tag{12.2}$$

Since the steady-state vector $u_f = u_0 \lim_{n\to\infty} P^n$, and taking matrix P^n (Table 12.9) and the initial state vector $u_0 = (0.142, \cdots, 0.142)$, we get the steady-state vector u_f.

12.1.3. Results

If we take the initial state vector $u_0 = (1/7, \cdots, 1/7)$, we get the steady-state vector u_f (Eq. 12.3).

$$u_f = (0.136, 0.081, 0.015, 0.015, 0.000, 0.015, 0.114) \tag{12.3}$$

When comparing u_0 (Eq. 12.4) with u_n (Eq. 12.3) we see that the diphthong with less probability has 0.000, while the others have equal probability 0.091.

$$u_0 = (0.142, 0.142, 0.142, 0.142, 0.142, 0.142, 0.142) \tag{12.4}$$

However, if we change the value of the initial state vector, see u_0 (Eq. 12.5), reducing the frequency of the diphthongs in the first third, the steady-state vector u_f (Eq. 12.6) shows an accumulation at the extremes of the vector u_f.

$$u_0 = (0.102, 0.102, 0.142, 0.142, 0.142, 0.182, 0.182) \tag{12.5}$$

$$u_f = (0.130, 0.079, 0.015, 0.015, 0.000, 0.015, 0.082) \tag{12.6}$$

If we change the value of the initial state vector u_0 (Eq. 12.7), reducing the frequency of the diphthongs in the last third, the steady-state vector u_f (Eq. 12.8) shows an increase at the opposite end of vector u_f.

$$u_0 = (0.182, 0.182, 0.142, 0.142, 0.142, 0.102, 0.102) \tag{12.7}$$

$$u_f = (0.143, 0.083, 0.015, 0.015, 0.000, 0.015, 0.146) \tag{12.8}$$

Finally, if we change matrix P isolating the diphthongs ea (Table 12.9), we can see a significant modification in the steady-state vector u_f (Eq. 12.10).

$$P = \begin{array}{c} \\ a \\ e \\ i \\ o \\ u \\ w \\ y \end{array} \begin{array}{c} \begin{array}{ccccccc} a & e & i & o & w & u & w \quad y \end{array} \\ \left(\begin{array}{ccccccc} 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 1.000 \\ 0.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.333 & 0.333 & 0.000 & 0.333 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \end{array} \right) \end{array} \tag{12.9}$$

$$u_f = (0.000, 0.354, 0.000, 0.000, 0.000, 0.000, 0.000) \tag{12.10}$$

CHAPTER 13

Computational Operations Research Issues

Abstract This chapter introduces Discrete and Continuous-Time Markov Chain Process aimed to predict the behavior of a waiting line, based on the probabilities of going from the state i to the state j, and also from velocity rates *lambda* and retracement *mu*. In both cases a numerical example is provided that shows the mechanics of both random walks as well as the pertinent observations when altering these parameters, and discusses the possibility of these parameters being altered in real time in an unsupervised algorithm.

Keywords: Conditional Probabilities, Initial State Vector, Markov Chain Process, Queuing Theory, Steady-State Vector, Transition Matrix

13.1. Queuing Theory-Discrete-Time Case

13.1.1. Instroduction

A waiting line [50] is a process inherent in many disciplines, its attention depends on whether or not other procedures can be concluded in opportunity, in this work the simple case is addressed on the possibility of advance or setback depends on the previous immediate experience. The Queuing Theory deals with the opportunity of an element in a waiting line to get a predetermined final state. This work is aimed to determine a Discrete-Time Markov Chain Process that simulates a waiting line where subject i transits from state E_i to state E_n (Fig. 13.2).

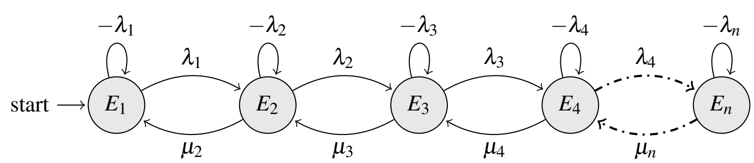

Figure 13.1: Geometrical representation of a waiting line with conditional probability rates for a discrete case.

13.1.2. Materials and Methods

To build the model, we have five states and the conditional probabilities p_{ij} represented by λ_i and μ_i (Table 13.1). Table 13.1 expresses the relative frequencies or transition rates from state i to state j.

Assume that the incidences expressed as conditional probabilities correspond to Table 13.1.

	E_1	E_2	E_3	E_4	E_i	E_n
E_1	$-\lambda$	λ	0.00	0.00	$\cdots$	1.00
E_2	$-\mu$	$\mu+\lambda$	μ	0.00	$\cdots$	1.00
E_3	0.00	$-\mu$	$\mu+\lambda$	μ	$\cdots$	1.00
E_4	0.00	0.00	$-\mu$	$\mu+\lambda$	μ	1.00
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
E_n	0.00	0.00	0.00	0.00	$\cdots$	1.00

Table 13.1: Conditional probabilities for the initial state (rows) and final state (columns).

The conditional probabilities in Table 13.1 were randomly built and they were used to build matrix P Eq. 13.1.

$$P = \begin{array}{c} \\ E_1 \\ E_2 \\ E_3 \\ E_4 \end{array} \begin{array}{c} \begin{array}{cccc} E_1 & E_2 & E_3 & E_4 \end{array} \\ \begin{pmatrix} -0.30 & 0.30 & 0.00 & 1.00 \\ -0.30 & 0.80 & 0.50 & 0.00 \\ 0.00 & -0.30 & 0.80 & 0.50 \\ 0.00 & 0.00 & 0.00 & 1.00 \end{pmatrix} \end{array} \tag{13.1}$$

Then, matrix P (Eq. 13.1) was multiplied by itself to get matrix P^5 (Eq. 13.7).

Note 13.1. For this calculation see Prog. A.13.

$$P^5 = \begin{array}{c} \\ E_1 \\ E_2 \\ E_3 \\ E_4 \end{array} \begin{array}{c} \begin{array}{cccc} E_1 & E_2 & E_3 & E_4 \end{array} \\ \begin{pmatrix} -0.02 & -0.10 & 0.08 & 1.00 \\ -0.10 & -0.43 & 0.14 & 1.19 \\ 0.05 & -0.09 & -0.38 & 1.41 \\ 0.00 & 0.00 & 0.00 & 1.00 \end{pmatrix} \end{array} \tag{13.2}$$

With the steady-state vector $u_f = u_0 \lim_{n\to\infty} P^n$, matrix P^n (Eq. 13.7), and the initial state vector $u_0 = (1.00, 0.00, 0.00, 0.00)$ we get the steady-state vector u_f.

13.1.3. Results

If we take the initial state vector $u_0 = (1.00, 0.00, 0.00, 0.00)$ we get the steady-state vector u_f Eq. 13.3

$$u_f = (0.003, -0.014, 0.002, 1.008) \tag{13.3}$$

When comparing u_0 (Eq. 13.4) with u_n (Eq. 13.3), we find that it gets to state E_4 in five units of time. Note that if we increase the accuracy, this state will be reached after seven or eight units of time.

$$u_0 = (1.000, 0.000, 0.000, 0.000) \tag{13.4}$$

However, if we alter the values of the initial state vector, see u_0 (Eq. 13.5), by reducing the frequency of the first state, the steady-state vector u_f (Eq. 13.6) shows an accumulation at the ends of vector u_f.

$$u_0 = (0.050, 0.350, 0.350, 0.250) \tag{13.5}$$

$$u_f = (0.006, -0.015, -0.022, 1.032) \tag{13.6}$$

Finally, if we alter the matrix P decreasing the value λ (Eq. 13.7), we see that the convergence to the last state is much longer. This can be seen in the values of the steady-state vector u_f for the fifth unit of time (Eq. 13.8)

$$P = \begin{array}{c} \\ E_1 \\ E_2 \\ E_3 \\ E_4 \end{array} \begin{array}{c} \begin{array}{cccc} E_1 & E_2 & E_3 & E_4 \end{array} \\ \begin{pmatrix} -0.10 & 0.10 & 0.00 & 1.00 \\ -0.10 & 0.90 & 0.20 & 0.00 \\ 0.00 & -0.10 & 0.90 & 0.20 \\ 0.00 & 0.00 & 0.00 & 1.00 \end{pmatrix} \end{array} \tag{13.7}$$

$$u_f = (0.004, -0.039, -0.034, 1.069) \tag{13.8}$$

13.1.4. Discussion

In my opinion, there is no better application scenario for the Markov Chain Process than to solve cases of waiting lines, for their pressing need to be solved. Daily we can see them either to provide supplies or some kind of service. Even the banking system has recently adopted the use of a “single queue” to improve the service.

Now, this is implemented in supermarkets that had a similar problem than Banks. How many cashiers had to be opened to satisfy the buyer’s demand? How to predict this demand to have the right numbers to optimize the service? This is a problem that can be successfully modelled by a Discrete-Time Markov Chain Process.

The elements of the matrix of transition probabilities P with the conditions in Table 13.1, correctly characterize a waiting line in discrete mode and the path to the end of the waiting line will depend on the values of λ y μ.

The Queuing theory is focused on the broad study of mathematical models on waiting lines. It does not solve the problem of getting a balance between the costs involved in the service and the waiting time to get the service. However, it provides valuable information to solve this problem.

The information it provides about the behaviour of the waiting line –if it is continuously growing or if it tends to stabilize–, the performance of the service, and the average waiting time makes it possible to characterize the scenario to study.

CHAPTER 14

Computational Information System Issues

Abstract This chapter defines a PageRank System for ranks web pages according to the transit detected in them. This simulation uses Discrete-Time and Continuous-Time Markov Chain Processes. For both approximations, numerical examples of both conditional probabilities and transition rate rates are provided. While both models are treated separately, in the end the desirability of designing a mixed network is discussed.

Keywords: Conditional Probabilities, Continuous-Time Markov Chain Process, Discrete-Time Markov Chain Process, Initial State Vector, Markov Chain Process, Steady-State Vector, PageRank System, Row-Vector of Final Conditions, Row-Vector of Initial Conditions, Transition Matrix

14.1. PageRank System - Discrete-Time Case

14.1.1. Instroduction

The attention of web pages [51, 52] is a topic of the recent discipline called Data Mining that seeks to position web pages by their demand for content. All web browsers aspire to be efficient in the opportunity to display the web pages with the most searched content. In this sense, a network scheme is proposed here for the attention of traffic between web pages. This chapter defines a network of Discrete-Time Markov Chain Processes (DMCP) that simulate internet page rank operators. These operators rank the web pages linked to them according to the demand or transit in that DMCP (Fig. 14.2).

In this sense, a Web pages Traffic Process is a Semi-Markov Process or Markov renewal process (Note 14.1)

Note 14.1. "Semi-Markovian processes provide a very flexible structure for modeling phenomena that evolve over time as they combine the probabilistic structure of a Markov chain and a renewal process. In other words, semi-Markovian processes model systems whose transitions between states occur according to a Markov chain and the times at which such transitions occur are random and form a process of renewal" [44].

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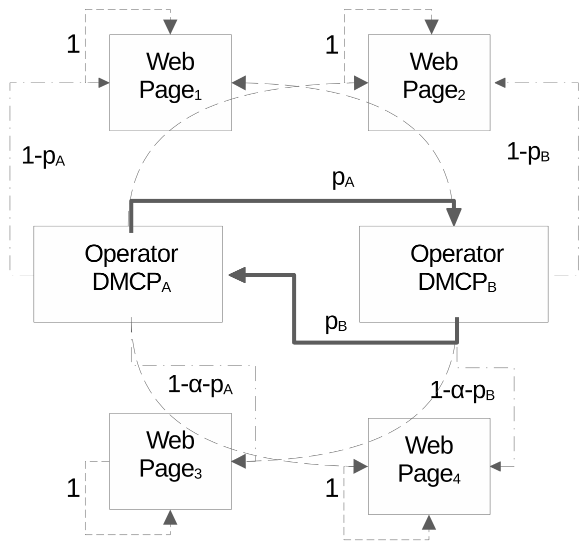

Figure 14.1: Network of Discrete-Time Markov Chain Processes.

14.1.2. Materials and Methods

To build the model we have two Discrete-Time Markov Chain Processes DMCP_A and (DMCP_B, four Web pages (Fig. 14.2), and the conditional probabilities p_{ij} for each one of them (Table 14.1) altered according to the increase in traffic from DMCP_A to DMCP_B.

$\cdots$	O_A	O_B	W_1	W_2	W_3	W_4
O_A	0	P_A	$1-P_A$	0	$1-\alpha-P_A$	0
O_B	P_B	0	0	$1-P_B$	0	$1-\alpha-P_B$
W_1	0	0	1	0	0	0
W_2	0	0	0	1	0	0
W_3	0	0	0	0	1	0
W_4	0	0	0	0	0	1

Table 14.1: Conditional probabilities p_{ij} of DMCP_i.

The conditional probabilities in Table 14.1 were randomly built and used to get matrix P (Eq. 14.1). Note that each DMCP_i has a matrix P and all of them have the same size.

$$P = \begin{array}{c} \\ O_A \\ O_B \\ W_1 \\ W_2 \\ W_3 \\ W_4 \end{array} \begin{array}{c} \begin{array}{cccccc} O_A & O_B & W_1 & W_2 & W_3 & W_4 \end{array} \\ \begin{pmatrix} 0 & P_A & 1-P_A & 0 & 1-\alpha-P_A & 0 \\ P_B & 0 & 0 & 1-P_B & 0 & 1-\alpha-P_B \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \tag{14.1}$$

Then, we multiply matrix P_i (Eq. 14.1) by itself to get matrix P_i^n, this will give the preference trend of the web pages.

Thus, the row-vector of final conditions $u_i^f = u_i^i \lim_{n\to\infty} P_i^n$ -where matrix P_i^n is matrix P multiplied n times by itself (Eq. 14.2)- is the row-vector of initial conditions, u_i^i is the vector that feeds the process DMCP$_i$, and the vector of final conditions u_i^f is the vector resulting from the process DMCP$_i$.

$$P^n = \begin{array}{c} \\ O_A \\ O_B \\ W_1 \\ W_2 \\ W_3 \\ W_4 \end{array} \begin{array}{c} \begin{array}{cccccc} O_A & O_B & W_1 & W_2 & W_3 & W_4 \end{array} \\ \begin{pmatrix} 0 & q_{12} & q_{13} & q_{14} & q_{15} & 0 \\ q_{21} & 0 & 0 & q_{24} & 0 & q_{26} \\ 0 & 0 & q_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & q_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & q_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \tag{14.2}$$

Probabilities P_a and P_B are altered as the result of the preference of each DMCP$_i$ in the web pages.

Note in Fig. 14.2 that once the four pages are ranked, the probability they stay there is 100%.

On the other hand, the two operators A and B are altered in their transition matrices, according to the preference for any of the web pages they connect. Note that each operator has communication with the four web pages and with both operators.

14.1.3. Discussion

This type of network makes it possible to orient the preferences of the operators to the web pages with more demand. Thus, it is possible to know and rank the web pages with each Discrete-Time Markov Chain Process.

You may have noticed when searching in a browser that the first ten web pages are the same if you repeat the search minutes later. This has to do directly with the search engines the browser uses.

However, if you do the same search one hour later, it is likely that the order of the web pages changes or that a new one appears.

This occurs because the search engine has a page rank system that will show the list of web pages that match the criteria programmed for that page rank.

One of the selection criteria used by the page rank system is to show the busiest (most searched) pages.

CHAPTER 15

Future Uses

Abstract This chapter makes a quick review of how the methods studied in this work, the Discrete and Continuous-Time Markov Chain Processes, can be applied to different fields and it explores their use con different approaches. It also examines how the applicability of these random walks can affect diverse disciplines with different impacts. The implementation of these methods can even have the option of self-learning programming.

Keywords: Algebra, Artificial Intelligence, Autonomous Decisions, Continuous Model, Deterministic Techniques, Differential System, Discrete Model, Discrete-Time Markov Chain Process, Granularity, Hidden Markov Model, Linear Algebra, Markov Chain Process, Matrix of Transition Probabilities, Matrix System, Network, Nodes, Partial Differential Equations, Patterns, Real Field, Real-Valued Functions, Stochastic Techniques, Structural Proteomics, Unsupervised Method, Vector-Valued Functions, Vertices

15.1. Scope

All disciplines use different techniques to recognize patterns. To categorize these techniques, we will divide them into deterministic and stochastic. The first group aims to construct real variable functions or vector functions to determine, with total precision, the location and time the variable occurs. The second group gives up precision and index the variable to a probable value for location and time.

However, sometimes precision places insuperable problems as a system of partial differential equations in the real field will not provide solutions due to the density of the field. On the other hand, a Discrete-Time Markov Chain Process is a matrix system where the number of rows or columns is the number of the variables involved.

Bearing this in mind, stochastic systems are much more efficient than deterministic ones in problems that involve multiple variables.

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15.2. Main Possibilities

There is a variation to a Markov Chain Process, the Hidden Markov Model, which is an indirect search for a determined pattern. Suppose we are looking to identify a regularity in an object and it cannot be isolated to search for it explicitly, however, it is known that it directly correlates with an observable regularity in another object, so the Hidden Markov Model searches the second observable pattern. This is an indirect search that widens the scope of the Markov Chain Process.

Particularly, some examples of the extension of the Markov Chain Process can be seen in these chapters.

Chap. 6 describes the procedure of a continuous model, and although getting its stabilization implies solving the problem with Linear Algebra its operation procedure is analogue to a discrete model which can be solved (Chap. 5) also with Linear Algebra.

Chap. 7 describes a problem of mobility between neighbourhoods within a city, in this problem, it is observed that it is feasible to build a computational network whose nodes turn out to be a Discrete or a Continuous-Time Markov Chain Process that can be solved in real-time so that the use of mixed models is possible.

Chap. 8 describes the use of the matrix of transition probabilities P as the profile searched, considering 16 elements to describe this profile. This case, besides showing the applicability in Structural Proteomics, shows the possibility of using different components of the Markov Chain Process as effective predictors or discriminants.

Chap. 9 introduces a model that studies three possible states of a financial share, in which the convenience of applying a Markov Chain Process to solve problems involving multiple variables is observed, and where differential systems or systems in differences are not practical.

Chap. 10 describes an extension of the Markov Chain Process, which makes it possible to address the nodes of network with different granularity . This network can also be implemented with vertices as differential systems and the Discrete-Time Markov Chain Process as nodes .

Chap. 11 The current pandemic caused by the SARS-CoV-2 virus shows the need for epidemiological systems focused on issuing early warnings for serious infections that affect the respiratory system. This is a multifactorial phenomenon that involves clinical and non-clinical variables. This profile shows that a Discrete and Continuous-Time Markov Chain Process network that is resolved in real time can be an efficient and unsupervised system that alerts medical authorities.

Chap. 12 The recognition of a language is very necessary before the emergence of computational lexicographic analysers since each grammar is different. In this case, it was observed that the use of diphthongs is a useful alternative to distinguish the language since adjustments to the algorithm can occur in real-time. Just as the grammatical structure of diphthongs is characteristic, another structure can be used as long as it is strongly associated with the language studied.

Chap. 13 studies a simple model of waiting lines, this is a problem that is faced in all scientific and non-scientific disciplines, and where the Markov Chain Process have turned out to be suitable for resolution. In that approach it was recommended a network of random walks that were solved and self-adjusted in real time, being this a viable and useful option.

Chap. 14 describes a way to rank web pages from the DMCPs transit dispatchers where the matrix of transition probabilities is altered. This is a problem related to massive information over the internet that requires very fast and efficient search engines, so the priority on the top web pages is the quality of their information instead of the payment of fees to place them there.

In all the cases of application reviewed in this work, it was found that it is feasible to strengthen the model by assigning them –as nodes of a network– that in turn can be self-modified from the results found in each self-evaluation, this way, it is possible to build an unsupervised method or ”artificial intelligence” to make autonomous decisions.

It should be noted that only if the long-term solution is required, it is necessary to carry out the algebraic operations. Otherwise, the Discrete-Time and Continuous-time Markov Chain Processes require defining the matrix and operating the simulation, so the model gets stabilized.

There are many other applications of the Markov Chain Process in different fields. This book aims to introduce the theory with application cases, motivating its use with the simplicity of the algebra involved and its ability to address multiple variables simultaneously.

There are many types of random walks [53, 54] equally efficient, however, the objective of this work has been covered with this compilation of cases.

SOLUTIONS

Solutions Chapter 1

Solution 1.1. (i) A third face coming up when tossing a double-face coin. (ii) Only one face appearing when tossing a double-face coin. (iii) Marking a different number in a pack of 20 cards, shuffle them and picking up one.

Solution 1.2. (i) $\Omega = \{\text{Side A, Side B}\}$. (ii) $A = \{\text{A}\}$. $B = \{\text{B}\}$. (iii) $P(A) = \frac{1}{2}$. $P(B) = \frac{1}{2}$.

Solution 1.3. If both events are dependent. (i) $P(A|B) = \frac{P(A\cap B)}{P(B)} = \frac{\frac{1}{5}}{\frac{1}{4}} = \frac{5}{4}$. (ii) $P(B|A) = \frac{P(A\cap B)}{P(A)} = \frac{\frac{1}{5}}{\frac{1}{3}} = \frac{5}{3}$. (iii) $P(A\cup B) = P(A) + P(B) - P(A\cap B) = \frac{1}{3} + \frac{1}{4} - \frac{1}{5}$.

Solution 1.4. i) E = Yellow, red, green ii) P(yellow) = 4/17; P(red) = 6/17; P(green) = 7/17.

Solution 1.5. The probability a person likes vanilla ice cream is $P(A)$. The probability a person likes chocolate ice cream is $P(B) = 0.50$. The probability a person likes vanilla and chocolate ice cream is $P(A\cup B) = 0.30$, so $P(A|B) = \frac{P(A\cap B)}{P(B)} = \frac{0.30}{0.50} = 0.60$.

Then, the probability a person likes vanilla ice cream, since he/she likes chocolate is $P(A|B)$ 60%.

Solution 1.6. We have to calculate $P(4|par)$. $P(4|par) = \frac{P(4\cap par)}{P(par)}$. Since $P(par) = 3/6 = 1/2$ and $P(4\cap par) =$ the probability that 4 and an even number come out is $= 1/6$. Then, $P(4|par) = (1/6)/(1/2) = 1/3$.

Solution 1.7. $P(B|A) = \frac{P(A\cap B)}{P(A)} = \frac{0.05}{0.025} = 0.020$, therefore, the conditioned probability is higher than the a priori probability (0.30). This is not always the case, sometimes the conditioned probability is equal or lower than the a priori probability.

Solution 1.8. See Eq.1.1

$$\begin{aligned} P(\mathrm{I}|\mathrm{D}) &= \frac{P(\mathrm{I}) \times P(\mathrm{D}|\mathrm{I})}{P(\mathrm{I}) \times P(\mathrm{I}|\mathrm{D}) + P(\mathrm{E}) \times P(\mathrm{E}|\mathrm{D}) + P(\mathrm{O}) \times P(\mathrm{O}|\mathrm{D})} \\ &= \frac{0.30 \times 0.85}{0.30 \times 0.85 + 0.30 \times 0.60 + 0.40 \times 0.30} \\ &= 0.46 \end{aligned} \tag{1.1}$$

Solution 1.9. Let A_1 be the event of "having an accident for high level of alcohol in blood", A_2 the event of "having an accident for careless driving", A_3 the event of "having an accident for other causes", and D the event of "having a fatal accident". Since the intersection of these events meet Bayes' theorem, the probability of having an accident for excessive alcohol intake is (Eq. 1.2).

$$\begin{aligned} P(A_1|D) &= \frac{P(A_1) \times P(D|A_1)}{P(A_1) \times P(D|A_1) + P(A_2) \times P(D|A_2) + P(\mathrm{O}) \times P(\mathrm{O}|\mathrm{D})} \\ &= \frac{0.60 \times 0.30}{0.60 \times 0.30 + 0.20 \times 0.20 + 0.20 \times 0.50} \\ &= 0.56 \end{aligned} \tag{1.2}$$

Solutions for Chapter 2

Solution 2.1. (i) Substituting in (Eq. 2.31)

$$u_t = u_0 e^{rt} \Leftrightarrow u_t = 30e^{9.9} \Leftrightarrow u_t = 597911.11 \tag{2.31}$$

Remark 2.1. Note that in three units of time the initial population 30 grew $\frac{597911}{30} \approx .19930$ times.

(ii) Substituting in (Eq. 2.32) $t = 0.21$

$$2u_0 = u_0 e^{rt} \Leftrightarrow 2 = e^{3.3t} \Leftrightarrow \ln 2 = 3.3t \Leftrightarrow \frac{\ln 2}{3.3} = t \tag{2.32}$$

Solution 2.2. (i)

$$u_1 = Pu_0 = \begin{pmatrix} 0.000 & 7.000 & 6.000 \\ 0.580 & 0.000 & 0.000 \\ 0.000 & 0.720 & 0.000 \end{pmatrix} \times \begin{pmatrix} 1.000 \\ 5.375 \\ 0.000 \end{pmatrix} = \begin{pmatrix} 37.62 \\ 0.58 \\ 03.87 \end{pmatrix} \tag{2.33}$$

(ii)

$$u_2 = Pu_1 = \begin{pmatrix} 0.000 & 7.000 & 6.000 \\ 0.780 & 0.000 & 0.000 \\ 0.000 & 0.720 & 0.000 \end{pmatrix} \times \begin{pmatrix} 37.62 \\ 0.58 \\ 03.87 \end{pmatrix} = \begin{pmatrix} 27.28 \\ 21.81 \\ 00.42 \end{pmatrix} \tag{2.34}$$

(iii)

$$u_3 = Pu_2 = \begin{pmatrix} 0.000 & 7.000 & 6.000 \\ 0.780 & 0.000 & 0.000 \\ 0.000 & 0.720 & 0.000 \end{pmatrix} \times \begin{pmatrix} 27.28 \\ 21.81 \\ 00.42 \end{pmatrix} = \begin{pmatrix} 111.22 \\ 13.27 \\ 11.22 \end{pmatrix} \tag{2.35}$$

(iv) There is no convergence in (i–iii).

Solution 2.3. See (Fig. 2.5)

APPENDICES

Appendix A
Computational Programs

Abstract This chapter presents the computational programs that were used to calculate all the automated processes in this book. These programs were developed in language Fortran 90 and Linux scripts.

A.1. One-dimensional random walk program

```
!       Author: Carlos Polanco
!       Date: July, 2022.
!
       IMPLICIT none

       INTEGER i, j
       INTEGER ifin
       DOUBLEPRECISION xi

    53 FORMAT  (f6.4,1x,A4)

!
!       Procedure to generates the random walk
       ifin = 1
       DO j = 1, 20
       CALL rnd001 (xi, i, ifin)
       IF (xi.ge.0.50) then
          WRITE (6, 53) xi, " - - - >"

       ELSE
          WRITE (6, 53) xi, "< - - - "
       ENDIF
       enddo

   200 CLOSE (1)
       STOP
       END
!
! Generation of random numbers
```

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```
!
      SUBROUTINE rnd001 (xi, i, ifin)
      INTEGER i, ifin
      DOUBLEPRECISION xi
      i = i * 54891
      xi = i * 2.328306e-10 + 0.5D00

      xi = xi * ifin
      END SUBROUTINE rnd001

      Input
c     None

      Output
      0.7181 --->
      0.9005 --->
      0.9302 --->
      0.5819 --->
      0.3915 <---
      0.0878 <---
      0.0049 <---
      0.1470 <---
      0.4478 <---
      0.4493 <---
      0.6186 --->
      0.5033 --->
      0.3815 <---
      0.2592 <---
      0.2323 <---
      0.3724 <---
      0.5112 --->
      0.9830 --->
      0.7876 --->
      0.8857 --->
```

A.2. Two-dimensional random walk program

```
!      Author: Carlos Polanco
!      Date: July, 2022.
!
      IMPLICIT none

      INTEGER i, j
      INTEGER ifin
      DOUBLEPRECISION xi

   53 FORMAT  (f6.4,1x,A5)

      ifin = 1
      DO j = 1, 20
!
!         Procedure to generates the two dimensional random walk
      CALL rnd001 (xi, i, ifin)
      IF (xi.ge.0.25) then
         WRITE (6, 53) xi, "Down"
      ENDIF
      IF (xi.ge.0.75) then
         WRITE (6, 53) xi, "Top"
      ENDIF

      IF ( (xi.ge.0.25) .and. (xi.le.0.50) ) then
         WRITE (6, 53) xi, "Left"
      ENDIF

      IF ( (xi.ge.0.50) .and. (xi.le.0.75) ) then
         WRITE (6, 53) xi, "Right"
      ENDIF
      enddo

  200 CLOSE (1)
      STOP
      END

!
!      Generation of random numbers

      SUBROUTINE rnd001 (xi, i, ifin)
      INTEGER i, ifin
      DOUBLEPRECISION xi
      i = i * 54891
      xi = i * 2.328306e-10 + 0.5D00

      xi = xi * ifin
      RETURN
      END SUBROUTINE rnd001
      Input
```

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SUBJECT INDEX

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