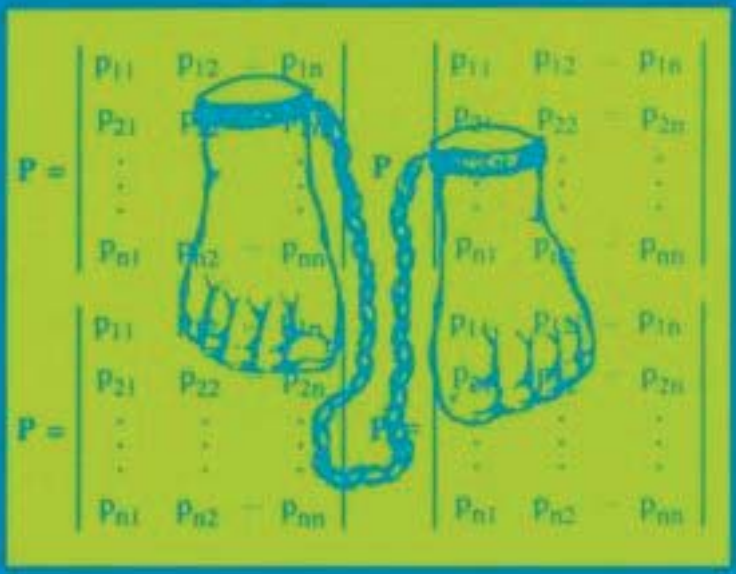
# Applications of Markov Chains in Chemical Engineering



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# PREFACE

Markov chains enable one to predict the *future* state of a *system* from its *present* state ignoring its *past* history.

Surprisingly, despite the widespread use of Markov chains in many areas of science and technology such as: Polymers, Biology, Physics, Astronomy, Astrophysics, Chemistry, Operations Research, Economics, Communications, Computer Networks etc., their applications in Chemical Engineering has been relatively meager.

A possible reason for this phenomenon might be that books containing material on this subject have been written in such a way that the simplicity of Markov chains has been shadowed by the tedious mathematical derivations. This caused one to abandon the book, thus loosing a potential tool for handling his problems.

There are many advantages, detailed in Chapter 1, of using the discrete Markov-chain model in Chemical Engineering. Probably, the most important advantage is that physical models can be presented in a unified description via *state vector* and a *one-step transition probability matrix.* Consequently, a process is demonstrated solely by the probability of a *system* to *occupy* a *state* or not to occupy it. William Shakespeare profoundly stated this in the following way: " **to be** (in a state) **or not to be** (in a state), **that is the question**".

I believe that Markov chains have not yet acquired their appropriate status in the Chemical Engineering textbooks although the method has proven very effective and simple for solving complex processes. Thus, the major objective of writing this book has been to try to change this situation. The book has been written in an easy and understandable form where complex mathematical derivations are abandoned. The demonstration of the fundamentals of Markov chains in Chapter 2 has been done with examples from the bible, art and real life problems. The majority of the book contains an extremely wide collection of examples viz.,

reactions, reactors, reactions and reactors as well as combined processes, including their solution and a graphical presentation of it. All this, to my opinion, demonstrates the usefulness of applying Markov chains in Chemical Engineering.

Bearing all the above in mind, leads me also to suggest this book as a useful textbook for a new course entitled *Applications of Markov chains in Chemical Engineering*.

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The most significant impact, however, has been that of my graduate students who participated in my course related to Markov chains. Their proclivity to ask 'why'? has forced me to rethink, recognize and rewrite many parts of the book again and again. In particular, many thanks are due to my student Adi Wolfson, who reviewed Chapter 2.

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Finally, since I have no co-authors, I must accept responsibility for all errors in this book.

Abraham Tamir

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**Chapter 0**

# BIBLICAL ORIGINS AND ARTISTIC DEMONSTRATIONS OF MARKOV CHAINS A HUMOROUS INTRODUCTION

The origin of Markov chains, a probabilistic model for predicting the *future* given the *present* of a process and ignoring its *past*, goes back to biblical times, i.e. to the Book of Books. This we know thanks to what has been said in Exodus 28, verse 13-14, "Make gold rosettes and two **CHAINS** of pure gold worked into a form of ropes, and fix them on the rosettes". A thorough investigation of this verse led to the conclusion that the word **CHAINS** is an abbreviation of **MARKOV CHAINS**. Thus, it turns out that Markov chains is a very old subject and, as said in Ecclesiastes 1 verse 9, "... And there is nothing new under the sun".

It is also surprising that available books [2-8, 15-18] related to the subject matter do not refer at all to biblical Markov processes. Such a process, for example, can be generated on the basis of Genesis 1 and is related to the order of the *days of the week* in the Creation. According to verse 27, *man* was created on Friday. The Bible describes this event very nicely as follows: " And God created *man* in His image, in the image of God he created him ... And there was evening and there was morning, the sixth day." Independent of the past history, i.e. Sunday to Friday, the probability that *man* will occupy a Saturday on the next day is 100%. In other words, since the present state is known, namely, Friday, and the probability of moving to the next state is also known, 100%, it is possible to predict Saturday as the future state of *man* with respect to the days of the week. The above example, elaborated later in example 2.11, demonstrates for the first time the essence of Markov chains proposed by Markov only in 1906 [1], much later than Biblical times.