Monte Carlo simulations of random variables, sequences and processes

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The main goal of analysis in this book are Monte Carlo simulations of Markov processes such as Markov chains (discrete time), Markov jump processes (discrete state space, homogeneous and non-homogeneous), Brownian motion with drift and generalized diffusion with drift (associated to the differential operator of Reynolds equation). Most of these processes can be simulated by using their representations in terms of sequences of independent random variables such as uniformly distributed, exponential and normal variables. There is no available representation of this type of generalized diffusion in spaces of the dimension larger than 1. A convergent class of Monte Carlo methods is described in details for generalized diffusion in the two-dimensional space.

CONTENTS

Chapter 1. Pseudo-random numbers

To simulate a random variable means to construct its numerical sample of an arbitrary large length. The basic idea is to represent the random variable in terms of one or more independent, uniformly distributed random variables. A random variable which is uniformly distributed in $[0, 1]$ is called the random number. Therefore, the construction of a numerical sample of the original random variable is transformed to a generation of a sample of random numbers. In this way the random number has an exclusive importance in simulations. The first chapter is devoted to a study of theoretical background of simulations of random numbers and to testing quality of simulated sequences. The existence of multiply equidistributed numbers and completely equidistributed numbers (=multiply equidistributed in Euclidean space of any dimension) is proved.

Chapter 2. Simulation of random variables

The main goal of this book is to describe basic ideas of Monte Carlo simulations of sample paths of stochastic processes. Therefore, it is natural to expect that this chapter is devoted to an analysis of Monte Carlo methods of simulations of those random variables (one-dimensional and multi-dimensional) which are often met in definitions of stochastic processes. Such random variables are the normal, exponential and Poisson variables.

Chapter 3. Simulation of stationary sequences

A stationary sequence of random variables is an important mathematical object in natural and technical sciences and it is necessary to develop methods of simulations of such objects. Only stationary sequences for which the singular part of the spectrum is absent are considered in this chapter. In other words the spectrum may have only the continuous and discrete components. Most of the results are formulated for stationary sequences of normal random variables. Apart from stationary sequences an important object in natural and technical sciences are random fields. Methods of simulation of fields on bounded domains in Euclidean spaces are also described. The problem of the estimation of a random field from data is discussed and methods of simulation are compared with widely exploited linear least square method.

Chapter 4. Simulation of Markov chains

In this chapter we begin to study Monte Carlo simulations of Markov processes. A natural first step in this program is Monte Carlo simulations of Markov chains because a Markov chain is a basic object in a study of homogeneous Markov processes. At the beginning, necessary objects for defining a Markov chain are described. Some additional properties about the structure of chains are given in exercises at the end of this chapter. The notion of the first exit from a permeable set is considered in details in the second section. Monte Carlo simulations of a class of Markov chains in an Euclidean space are studied in the third section. Some problems with the first exit from permeable sets of Markov chains are considered in the fourth section. Problems are solved in terms of deterministic methods as well as Monte Carlo methods and results are compared. Two walkers meeting model defined in terms of two Markov chains in the same state space is particularly interesting. Numerical methods for this model are analyzed in more details from the standpoint of deterministic evaluation and Monte Carlo prediction of certain statistical moments. If an initial value problem for a system of linear differential equations (IVP for ODE) has the system matrix with compartmental structure, Markov chains can be simply related to a class of numerical methods for solving ODE. This fact underlines an importance of Markov chains in applications in natural and technical sciences. A class of numerical methods for ODE, which are directly related to Markov chains, are described in the fifth section.

Chapter 5. Simulation of Markov jump processes

A simulation of a homogeneous Markov jump process can be carried out by a simple numerical procedure which is based on the representation of process in

terms of a chain and a sequence of independent exponential random variables. On the other hand a simulation of a non-homogeneous Markov jump process can be a complex numerical process. The time interval of observation must be discretized by a grid and then instead of handling with the original non-homogeneous process one has to consider and simulate some of its approximations by a non-homogeneous Markov chain on the same state space. The distributions of chain for defined discrete times in grid must be calculated from an initial value problem for ODE. There are non-homogeneous processes which can be transformed to homogeneous ones by using a transformation of time. Such processes are also studied here with certain extent.

A relation between Markov jump processes and initial value problems for ODE gives us a possibility to estimate solutions to ODE by using M.C. methods. This numerical approach to an estimation of solutions to initial value problems for ODE is discussed in the last section of this chapter.

In chapters on simulation of Brownian motion and generalized diffusion Markov jump processes play an essential role with regard to the problem of approximations of these processes. Very often a Markov jump process in such discussion and formulation of results is denoted by MJP.

Chapter 6. Simulation of Brownian motion

In the previous chapter IVPs for ODE and Markov jump process are mutually related, the connection being the fundamental solutions of ODE and the transition densities of MJPs. This interrelation between differential equations and stochastic processes is generalized in this chapter to another pair of objects, the first being the heat equation and the second one is a stochastic process which is called Brownian motion. The object which connects the heat equation and Brownian motion is the fundamental solution of heat equation. Again, the fundamental solution is interpreted as the transition probability of considered process. A heat equation can be approximated arbitrarily well by IVPs for ODE. A consequence of this fact is a possibility to approximate Brownian motion by a sequence of MJPs.

Simulation of Brownian motion without drift is a simple numerical process which is based on simulation of normal random variables. For simulation of Brownian motion with drift it is necessary to approximate the process accordingly and simulate the approximations. Two methods are described and illustrated by examples. One method is based on approximations of the corresponding stochastic differential equation and the other one is based on approximations of the process with MJPs.

The exits from permeable sets are considered in more details. The expectation and variance of the first exit time are expressed in terms of solutions of certain BVPs and IVPs. The efficiency of estimation of statistical moments of the first exit time and related random variables by using Monte Carlo methods is demonstrated in examples. Methods of simulation which are based on discretizations of stochastic differential equations are simpler than those ones which are based on approximating MJPs. However, better results can be obtained by the latter methods. Deterministic methods of estimations are used for comparison.

Chapter 7. Simulation of generalized diffusion

The law of spreading of heat in an isotropic medium is given by the heat equation. Heat equation and Brownian motion are mutually related, connection between the two objects being the fundamental solution of heat equation. Spreading of heat in an anisotropic medium is defined by a parabolic differential equation with anisotropic diffusion. This equation is related to another stochastic process which is called generalized diffusion. The bridge connecting two mathematical objects is the fundamental solution of anisotropic diffusion equation.

A Brownian motion can be represented by SDE, i.e. by a mathematical object which is not related a priori to heat equation. Therefore, we can simulate a Brownian motion by two genuinely different methods, one is based on discretization of SDE, and the other is based on approximations of Brownian motion by MJPs. A

generalized diffusion in $\mathbb{R}^d, d > 1$, does not have a representation in terms of SDE or similar objects. In order to simulate generalized diffusion we have to construct a sequence of MJPs approximating it and simulate the approximations.

In this chapter we develop a method for simulation of generalized diffusion. The method is based on approximations of generalized diffusion by a sequence of MJPs in grids of $\mathbb{R}^d$. For generalized diffusion in $\mathbb{R}^2$ the construction of MJPs is relatively simple. Therefore, methods of simulations are developed in details only for generalized diffusion in $\mathbb{R}^2$.

The stochastic processes of previous chapters are defined explicitly in terms of independent random numbers. For the generalized diffusion this approach is not possible. In order to introduce the processes of this chapter in a plausible way certain amount of new analytical tools is necessary to use.