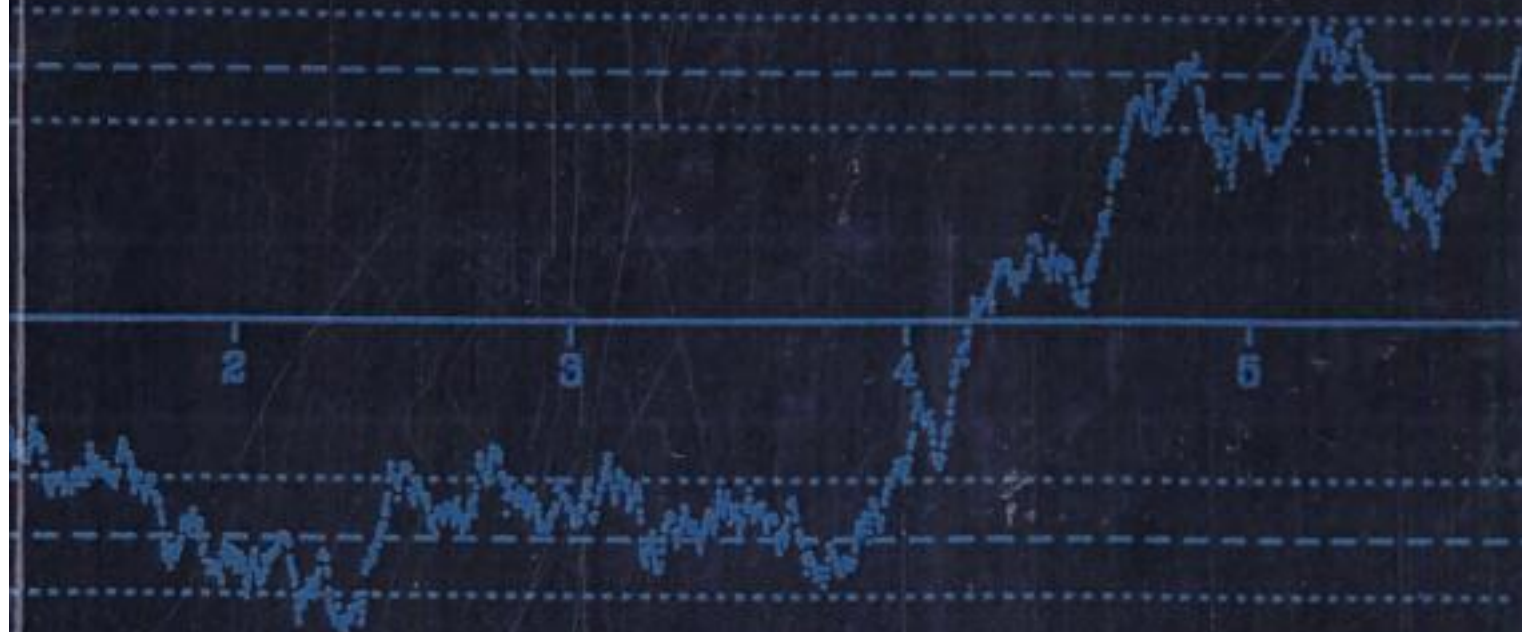


# MARKOV PROCESSES

AN INTRODUCTION FOR  
PHYSICAL SCIENTISTS



DANIEL T. GILLESPIE

Markov Processes: An Introduction for Physical Scientists, Daniel T. Gillespie, Gulf Professional Publishing, 1992, 0122839552, 9780122839559, 565 pages. Markov process theory is basically an extension of ordinary calculus to accommodate functions whose time evolutions are not entirely deterministic. It is a subject that is becoming increasingly important for many fields of science. This book develops the single-variable theory of both continuous and jump Markov processes in a way that should appeal especially to physicists and chemists at the senior and graduate level. Key Features\* A self-contained, pragmatic exposition of the needed elements of random variable theory\* Logically integrated derivations of the Chapman-Kolmogorov equation, the Kramers-Moyal equations, the Fokker-Planck equations, the Langevin equation, the master equations, and the moment equations\* Detailed exposition of Monte Carlo simulation methods, with plots of many numerical examples\* Clear treatments of first passages, first exits, and stable state fluctuations and transitions\* Carefully drawn applications to Brownian motion, molecular diffusion, and chemical kinetics.

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Markov process theory is basically an extension of ordinary calculus to accommodate functions whose time evolutions are not entirely deterministic. It is a subject that is becoming increasingly important for many fields of science. This book develops the single-variable theory of both continuous and jump Markov processes in a way that should appeal especially to physicists and chemists at the senior and graduate level.

I have read and worked through much of Gillespie's book. It was exactly what I needed in the way of a meaty but clear and accessible introduction to the subject. I know of no other book like it. There are good books that are more mathematically oriented (Okesendahl), that outline rather than narrate (Gardiner), and that introduce a more limited content (my own), but there is nothing like Gillespie's book: introductory yet wide-ranging content. It was perfect for this physicist who wanted to be introduced to the details of the subject.

approximate average birth-death Markov process Brownian motion calculate Chapman-Kolmogorov equation characterizing functions  $A(x,t)$  collisions constant continuous Markov process deduce defined in Eq definition derive differential equation diffusion function Dirac delta function evidently evolution equations exponential Fokker-Planck equation follows from Eq gas molecule given homogeneous jump Markov homogeneous Markov process implies infinitesimal initial condition integrand interval joint density function jump Markov process Kramers-Moyal equation labeled molecule Langevin equation Markov process  $X(t)$  Markov state density master equation microstates normal random variable  $\sigma(dt)$  obtain one-standard deviation envelope Ornstein-Uhlenbeck process  $P_a(n)$   $P_a(x)$  parameter particle peak plot Poisson process probability process with characterizing propagator density function propagator moment functions radioactive decay relative maximum result  $S(dt)$  sample values satisfies Section side of Eq simulation algorithm solution standard deviation stationary Markov statistically independent stochastic stochastic process Subsection substituting theorem time-evolution equations uniform random number unit uniform random variance and covariance velocity  $W_+(n)$  Wiener process zero

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Book Description: Elsevier Science, 1991. Hardback. Book Condition: New. 9.02 by 5.98 inches. (592 pages) This item is printed on demand. Please allow up to 10 days extra for printing & delivery. Markov process theory is basically an extension of ordinary calculus to accommodate functions whose time evolutions are not entirely deterministic. It is a subject that is becoming increasingly important for many fields of science. This book develops the single-variable theory of both continuous and jump Markov processes in a way that should appeal especially to physicists and

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**Key Features**

- \* A self-contained, pragmatic exposition of the needed elements of random variable theory
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**Random Variable Theory. General Features of a Markov Process. Continuous Markov Processes. Jump Markov Processes with Continuum States. Jump Markov Processes with Discrete States. Temporally Homogeneous Birth-Death Markov Processes. Appendixes: Some Useful Integral Identities. Integral Representations of the Delta Functions. An Approximate Solution Procedure for Open Moment Evolution Equations. Estimating the Width and Area of a Function Peak. Can the Accuracy of the Continuous Process Simulation Formula Be Improved? Proof of the Birth-Death Stability Theorem. Solution of the Matrix Differential Equation. Bibliography. Index.**

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Daniel Thomas Gillespie (born 1938) is a physicist who is best known for his derivation in 1976 of the stochastic simulation algorithm (SSA), also called the Gillespie algorithm.[1][2] The SSA is a procedure for numerically simulating the time evolution of the molecular populations in a chemically reacting system in a way that takes account of the fact that molecules react in whole numbers and in an essentially random way. Since the late 1990s, the SSA has been widely used to simulate chemical reactions inside living cells, where the small molecular counts of some reactant species often invalidate the differential equations of traditional deterministic chemical kinetics.

Gillespie's original derivation of the SSA[1] began by considering how chemical reactions actually occur in a well-stirred dilute gas. Reasoning from physics (and not by heuristically extrapolating deterministic reaction rates to a stochastic context), he showed that the probability that a specific reaction will occur in the next very small time  $dt$  could be written as an explicit function of the current species populations multiplied by  $dt$ . From that result he deduced, using only the laws of probability, an exact formula for the joint probability density function  $p(\vec{I}_{t+dt}, j)$  of the time  $\vec{I}_{t+dt}$  to the next reaction event and the index  $j$  of that reaction. The SSA consists of first generating random values for  $\vec{I}_{t+dt}$ , and  $j$  according to  $p(\vec{I}_{t+dt}, j)$ , and then actualizing the next reaction accordingly. The generating step of the SSA can be accomplished using any of several different methods, and Gillespie's original paper[1] presented two: the "direct method", which follows from a straightforward application of the well known Monte Carlo inversion method for generating random numbers; and the "first-reaction method", which is less straightforward but mathematically equivalent. Later workers derived additional methods for generating random numbers according to Gillespie's function  $p(\vec{I}_{t+dt}, j)$  which offer computational advantages in various specific situations. Gillespie's original derivation of the SSA[1][2][3] applied only to well-stirred dilute gas systems. It was widely assumed/hoped that the SSA would also apply when the reactant molecules are solute molecules in a well-stirred dilute

solution with many smaller solvent molecules. In fact it does, but that was not definitively established until 2009.[4] The extent to which the SSA is valid under other typical cellular conditions, such as when the reactant molecules crowd each other or when they move by active transport mechanisms along physically confined pathways, remains to be seen.

Gillespie received his Ph.D. from Johns Hopkins University in 1968 with a dissertation in experimental elementary particle physics under Aihud Pevsner. Part of his dissertation derived procedures for stochastically simulating high-energy elementary particle reactions using digital computers, and Monte Carlo methodology would play a major role in his later work. During his graduate student years at JHU he was also a Jr. Instructor (1960–63) and an Instructor (1966-68) in the sophomore General Physics course.

From 1971 to 2001, Gillespie was a civilian scientist at the Naval Weapons Center in China Lake, California. Initially he was a Research Physicist in the Earth and Planetary Sciences Division. There his research in cloud physics led to a procedure for simulating the growth of raindrops in clouds,[14] and that prompted his paper on the SSA.[1] In 1981 he became Head of the Research Department's Applied Mathematics Research Group, and in 1994 he was made a Senior Scientist in the Research Department.

Since his retirement from China Lake in 2001, Gillespie has been a private consultant in computational biochemistry, working under contract for various periods of time with the California Institute of Technology, the Molecular Sciences Institute (in Berkeley), the Beckman Institute (at Caltech), and the University of California, Santa Barbara. Most of this work has been, and continues to be, in collaboration with the Linda Petzold research group in the Computer Sciences Department of UCSB.

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