SS 2011 (27. + 28. KW)

Stochastische Markov-Prozesse

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A) Master-Gleichung
(Chapman-Kolmogorov Gl.)

B) Fokker-Planck-Gleichung
(FPE)

C) Langevin Gleichung

Irreversibilität

Nichtgleichgewicht ⟶ Gleichgewicht

mittel Zufallsprozesse

[Brownsche Bewegung, Diffusion, chem. Reaktionen, Absorbierende/Reflektierende Grenzen]

Statistische Physik / 05.07.2011 / R. M. ①

Siehe: Physics of Stochastic Processes von R. Mahnke u.a. Wiley, 2009, Kap. 3

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3 Master Equation

3.1 Markovian Stochastic Processes

Stochastic processes enter into many physical descriptions of nature. Historically first the motion of a heavy particle in a fluid of light molecules has been observed. The path of such *Brownian particle* consists of stochastic displacements due to random collisions. Such motion was studied by the Scottish botanist Robert Brown (1773 – 1858). In 1828 he discovered that the microscopically small particles into which the pollen of plants decay in an aqueous solution are in permanent irregular motion. Such a stochastic process is called *Brownian motion* and can be interpreted as discrete random walk or continuous diffusion movement. This topic is considered in textbooks about Statistical Physics [38,85,194,206,213] as well as in many books or monographs about stochastic processes [6,25,55,84,121,156,160,172,201,211,234].

The intuitive background to describe the irregular motion completely as stochastic process is to measure values $x_1, x_2, \ldots, x_n, \ldots$ at time moments $t_1, t_2, \ldots, t_n, \ldots$ of a time dependent random variable $x(t)$ and assume that a set of joint probability densities, called JPD–distributions

gemeinsame

$$p_n(x_1,t_1;x_2,t_2;\ldots;x_n,t_n)\,, \qquad n=1,2,\ldots \tag{3.1}$$

exists. The same can be done by introducing the set of conditional probability densities (called CPD–distributions)

bedingte Wahrscheinlichkeitsdichten

$$p_n(x_n,t_n \mid x_{n-1},t_{n-1};\ldots;x_1,t_1)\,, \qquad n=2,3,\ldots \tag{3.2}$$

denoting that at time t_n the value x_n can be found, if at previous times $t_{n-1},\ldots,t_1$ the respective values $x_{n+1},\ldots x_1$ were present. The relationship between JPD and CPD is given by

$$p_{n+1}(x_1,t_1;\ldots;x_{n+1},t_{n+1}) = p_{n+1}(x_{n+1},t_{n+1} \mid x_n,t_n;\ldots;x_1,t_1)\; p_n(x_1,t_1;\ldots;x_n,t_n)\,. \tag{3.3}$$

Physics of Stochastic Processes. R. Mahnke et al.

ISBN: 3-527-XXXXX-X, April 11, 2008

This stochastic description in terms of macroscopic variables will be called *mesoscopic*. Why? Typical systems encountered in the everyday life like gases, liquids, solids, biological organisms, human or technical objects consist of about 10^{23} interacting units. The macroscopic properties of matter are usually the result of collective behavior of a large number of atoms and molecules acting under the laws of quantum mechanics. To understand and control these collective macroscopic phenomena the complete knowledge based upon the known fundamental laws of microscopic physics is useless because the problem of interacting particles is much beyond the capabilities of the largest recent and future computers. The understanding of complex macroscopic systems consisting of many basic particles (in the order of atomic sizes: 10^{-10} m) requires the formulation of new concepts. One of the methods is the stochastic description taking into account the statistical behavior. Since the macroscopic features are averages over time of a large number of microscopic interactions, the stochastic description links both approaches together, the microscopic and the macroscopic one, to give probabilistic results. Monographs (recommended for physicists and engineers) devoted to stochastic concepts are mainly written as advanced courses on Statistical Physics like that by Josef Honerkamp [85] and on Statistical Thermodynamics by Werner Ebeling & Igor M. Sokolov [38], or well–known textbooks on Stochastic Processes, see e. g. [6] by Vadim S. Anishenko et al., [55] by Crispin W. Gardiner, [84] by Josef Honerkamp, [234] by N. G. van Kampen.

Speaking about a *stochastic process* from the physical point of view we always refer to stochastic variables (random events) changing in time. A realization of a stochastic process is a trajectory $x(t)$ as function of time. Here we introduce a hierarchy of *probability distributions*

$$p_n(x_1,t_1;x_2,t_2;\ldots;x_n,t_n)\,dx_1dx_2\ldots dx_n\,, \qquad n=1,2,\ldots\,, \tag{3.4}$$

where $p_1(x_1,t_1)dx_1$ is known as time dependent probability of first order to measure the value x_1 (precisely, the value within $[x_1, x_1+dx_1]$) at time t_1, $p_2(x_1,t_1;x_2,t_2)$ is the same probability of second order, up to higher–order joint distributions $p_n(x_1,t_1;\ldots;x_n,t_n)dx_1dx_2\ldots dx_n$ to find for the stochastic variable the value x_1 at time moment t_1, the value x_2 at time t_2 and so on. Only the knowledge of such infinite hierarchy of joint probability densities $p_n(x_1,t_1;\ldots;x_n,t_n)$ (expression (3.1)) with $n=1,2,\ldots$ gives us the overall description of the stochastic process.

A stochastic process without any dynamics (like a coin throw or any hazard game) is called a temporally *uncorrelated process*. It holds that

$$p_2(x_1,t_1;x_2,t_2) = p_1(x_1,t_1)\,p_1(x_2,t_2)\,, \tag{3.5}$$

if random variables at different times are mutually independent. It means that each realization of a random number at time t_2 does not depend on previous

time t_1, i. e., the correlation at different times $t_1 \neq t_2$ is zero. Such a stochastic process, where function $p_1(x_1,t_1) \equiv p_1(x)$ is the density of a normal distribution, is called *Gaussian white noise*. The Gaussian white noise with its rapidly varying, highly irregular trajectory is an idealization of a realistic fluctuating quantity. Due to factorization of all higher–order joint probability densities the knowledge of the normalized distribution $p_1(x_1,t_1)$ describes the process totally.

Now we are introducing dynamics via correlations between two different time moments. This basic assumption enables us to define the *Markov process*, also called *Markovian process*, by two quantities totally, namely the first–order $p_1(x_1,t_1)$ and the second–order probability density $p_2(x_1,t_1;x_2,t_2)$, or equivalently by the joint probability $p_1(x_1,t_1)$ and the conditional probability $p_2(x_2,t_2 \mid x_1,t_1)$ to find the value x_2 at time t_2, given that its value at previous time t_1 $(t_1 < t_2)$ is x_1. In contradiction to uncorrelated processes (3.5) discussed before, Markov processes are characterized by the following temporal relationship

$$p_2(x_1,t_1;x_2,t_2) = p_2(x_2,t_2|x_1,t_1)\, p_1(x_1,t_1)\,. \tag{3.6}$$

The *Markov property*

$$p_n(x_n,t_n \mid x_{n-1},t_{n-1};\ldots;x_1,t_1) = p_2(x_n,t_n \mid x_{n-1},t_{n-1}) \tag{3.7}$$

enables us to calculate all higher–order joint probabilities p_n for $n > 2$. To determine the fundamental equation of stochastic processes of Markov type we start with the third–order distribution $(t_1 < t_2 < t_3)$

$$\begin{aligned} p_3(x_1,t_1;x_2,t_2;x_3,t_3) &= p_3(x_3,t_3 \mid x_2,t_2;x_1,t_1)\, p_2(x_1,t_1;x_2,t_2) \\ &= p_2(x_3,t_3 \mid x_2,t_2)\, p_2(x_2,t_2 \mid x_1,t_1)\, p_1(x_1,t_1) \end{aligned} \tag{3.8}$$

and integrate this identity over x_2 and divide both sides by $p_1(x_1,t_1)$. We get the following result for the conditional probabilities defining a Markov process

$$p_2(x_3,t_3 \mid x_1,t_1) = \int p_2(x_3,t_3 \mid x_2,t_2)\, p_2(x_2,t_2 \mid x_1,t_1)\, dx_2\,, \tag{3.9}$$

called *Chapman–Kolmogorov equation*.

As already stated the Markov process is uniquely determined through the distribution $p_1(x,t)$ at time t and the conditional probability $p_2(x',t' \mid x,t)$, also called transition probability from x at t to x' at later t', to determine the whole hierarchy p_n $(n \geq 3)$ by the Markov property (3.7). Also these two functions cannot be chosen arbitrarily, they have to fulfill two consistency conditions, namely the Chapman–Kolmogorov equation (3.9)

$$p_2(x'',t'' \mid x,t) = \int p_2(x'',t'' \mid x',t')\, p_2(x',t' \mid x,t)\, dx'\,, \tag{3.10}$$

the Markov relationship (3.6)

$$p_1(x',t') = \int p_2(x',t'|x,t)\, p_1(x,t)\, dx\,, \tag{3.11}$$

and the normalization condition

$$\int p_1(x',t')\, dx' = 1\,. \tag{3.12}$$

The history in a Markov process, given by (3.7), is very short, only one time interval from t to t' plays any role. If the trajectory has reached x at time t, the past is forgotten, and it moves toward x' at t' with a probability depending on x,t and x',t' only. The entire information relevant for the future is thus contained in the present. A Markov process is a stochastic process for which the future depends on the past and the present only through the present. It has no memory [201]. In an ordinary case where the space of states x is locally homogeneous this gives sense to transform the Chapman–Kolmogorov equation (3.9) in an equivalent differential equation in the short time limit $t' = t+\tau$ with small τ tending to zero. The short time behavior of the transition probability $p_2(\cdot \mid \cdot)$ should be written as series expansion with respect to time interval τ in the form

$$p_2(x,t+\tau \mid x'',t) = [1 - \bar{w}(x,t)\tau]\,\delta(x-x'') + \tau w(x,x'',t) + \mathcal{O}(\tau^2)\,. \tag{3.13}$$

The new quantity $w(x,x'',t) \geq 0$ is the transition rate, the probability per time unit, for a jump from x'' to $x \neq x''$ at time t. This transition rate w multiplied by the time step τ gives the second term in the series expansion describing transitions from another state x'' to x. The first term (with the delta function) is the probability that no transitions takes place during time interval τ. Based on the normalization condition

$$\int p_2(x,t+\tau \mid x'',t)\, dx = 1 \tag{3.14}$$

it follows that

$$\bar{w}(x,t) = \int w(x'',x,t)\, dx''\,. \tag{3.15}$$

The ansatz (3.13) implies that a realization of the random variable after any time interval τ retains the same value with a certain probability or attains a different value with the complementary probability. A typical trajectory $x(t)$ consists of straight lines $x(t) = \text{const}$ interrupted by jumps. An illustration is presented in Fig. 3.1 .

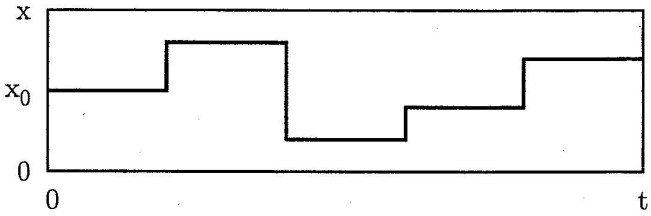

Fig. 3.1 Sketch of time evolution of a stochastic one–dimensional variable $x(t)$. The stochastic trajectory consists of pieces of deterministic motion interrupted by jumps.

From Chapman–Kolmogorov equation (3.9) together with (3.13) we get

$$\begin{aligned} p_2(x,t+\tau \mid x',t') &= \int p_2(x,t+\tau \mid x'',t)p_2(x'',t \mid x',t')\,dx'' \\ &= \int [1-\bar{w}(x,t)\tau]\,\delta(x-x'')p_2(x'',t \mid x',t')\,dx'' \\ &\quad + \int \tau w(x,x'',t)p_2(x'',t \mid x',t')\,dx'' + \mathcal{O}(\tau^2)\,. \end{aligned} \tag{3.16}$$

With (3.15) and after taking the short time limit $\tau \to 0$ one obtains the following differential equation

$$\frac{\partial}{\partial t}p_2(x,t \mid x',t') = \int w(x,x'',t)p_2(x'',t \mid x',t')\,dx'' - \int w(x'',x,t)p_2(x,t \mid x',t')\,dx''\,. \tag{3.17}$$

In order to rewrite the derived equation in a form well known in physical concepts we get after multiplication by $p_1(x',t')$ and integration over x' the differential formulation of the Chapman–Kolmogorov equation

$$\frac{\partial}{\partial t}p_1(x,t) = \int w(x,x',t)p_1(x',t)\,dx' - \int w(x',x,t)p_1(x,t)\,dx' \tag{3.18}$$

called *master equation* in the (physical) literature.

The name 'master equation' for the above probability balance equation is used in a sense that this differential expression is a general, fundamental or basic equation. For a homogeneous in time process the transition rates $w(x,x',t)$ are independent of time t and therefore $w(x,x',t) = w(x,x')$. The short time transition rates w have to be known from the physical context, often like an intuitive ansatz, or have to be formulated based on a reasonable hypothesis or approximation. One of them is *Fermi's golden rule* originating from microscopic quantum theory [194]. With known transition rates w and given initial distribution $p_1(x,t=0)$ the master equation (3.18) gives the resulting evolution of the probability p_1 over an infinitely long time period.

The well–known master equation can be written in different ways. Besides the continuous formulation with one variable x the generalization to the multi–dimensional as well as discrete case is obvious. Instead of $p_1(x,t)$ with the high–dimensional probability vector $P(\underline{x},t) \equiv P(x_1, x_2, \cdots, x_n, t)$ we may write the master equation in the discrete form (with summation instead of integration) as

$$\frac{\partial}{\partial t} P(\underline{x},t) = \sum_{\underline{x}' \neq \underline{x}} \{w(\underline{x},\underline{x}')P(\underline{x}',t) - w(\underline{x}',\underline{x})P(\underline{x},t)\} \ . \tag{3.19}$$

Generalizations of the master equation has been developed by Honerkamp and Breuer [85], Montroll and West [165] and others. To perform stochastic simulations of complex systems like piecewise deterministic Markov processes, stochastic formulation of fluid dynamics or reaction–diffusion equations the so–called many–body or multivariate master equation have been introduced. To describe quantum random systems the master equation is usually called Pauli master equation.

3.2 The Master Equation

The basic equation of stochastic Markov processes, called *master equation* or explicitly *forward master equation*, is usually written as gain–loss equation (3.18) for the probabilities $p(x,t)$ in the form

$$\frac{\partial p(x,t)}{\partial t} = \int \{w(x,x')p(x',t) - w(x',x)p(x,t)\}\, dx' \ . \tag{3.20}$$

This very general equation can be interpreted as local balance for the probability densities which have to fulfill the global normalization condition

$$\int p(x,t)\, dx = 1 \tag{3.21}$$

at each time moment t, also at the beginning for the initial distribution $p(x, t = 0)$. The linear master equation (3.20) with known transition rates per unit time $w(x,x')$ is a so–called Markov evolution equation showing the relaxation from a chosen starting distribution $p(x, t = 0)$ to some final probability distribution $p(x, t \to \infty)$. The linearity of the master equation is based on the assumption that the underlying dynamics is Markovian. The transition probabilities w do not depend on the history of reaching a state, so that the transition rates per unit time are indeed constants for a given temperature or total energy.

If the state space of the stochastic variable is a discrete one, often considering natural numbers within a finite range $0 \leq n \leq N$, the master equation for