A direct numerical method for obtaining the counting statistics for stochastic processes

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Abstract. We propose a direct numerical method for calculating the statistics for the numbers of transitions in stochastic processes, without having to resort to Monte Carlo calculations. The method is based on a generating function method, and arbitrary moments of the probability distribution of the number of transitions are in principle calculated by solving numerically a system of coupled differential equations. As an example, a two-state model with a time-dependent transition matrix is considered and the first, second and third moments of the current are calculated. This calculation scheme is applicable for any stochastic process with a finite state space, and it would be helpful for studying current statistics for nonequilibrium systems.

Keywords: stochastic particle dynamics (theory), dynamics (theory), current fluctuations

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1. Introduction

The statistics of nonequilibrium currents has attracted the interest of many physicists (for example, see [1]). The statistical information is related to the counting of the numbers of specific transitions in stochastic processes, and these problems have been widely studied in physics and chemistry [2]–[8]. A general scheme for counting the number of transitions, i.e., obtaining the counting statistics, has been recently developed (e.g., [5]), and various exact and approximate analytical results have been found. For example, a stochastic system under periodic perturbations can exhibit a net current, a so-called pump current, and it has been shown that this pump current is related to the geometric phase [9]–[11]. For the adiabatic case in which the changes of the periodic perturbations are very slow, an analysis with the aid of the Berry phase is valid, and analytical expressions for the current (the first moment) and variance have been obtained for a specific case [9]. However, to confirm these analytical expressions, Monte Carlo calculations have been performed; to be precise, although the first moment can be calculated from solutions of the master equation, Monte Carlo calculations were needed in order to estimate the variance numerically [9]. Although numerical simulations are helpful for studying such time-dependent systems, Monte Carlo calculations can become very costly, as discussed in [9].

In the present paper, we derive a direct numerical method for calculating moments of the probability distribution of the number of specific transitions in a stochastic process. Although a numerical method for calculating photon emission statistics has been proposed recently [12], the method has only been applied to quantum systems. We will discuss in the following, with the aid of the generating function approach developed by Gopich and Szabo [5], a numerical method that applies to classical stochastic processes and in which the numerical effort required to obtain the moments of the probability distribution reduces to integrating numerically a system of coupled differential equations. That is, this numerical method does not involve Monte Carlo type calculations. In principle, it is possible to apply the numerical method to a system with a finite state space, such as the photon statistics in a single-molecule system [5]. In addition, the method is applicable to a system under arbitrary time-dependent perturbations. It would be difficult in general to obtain analytic expressions for current statistics under complicated time-dependent perturbations. Hence, the direct numerical method will be useful for investigations of
current statistics in nonequilibrium systems, such as a symmetric exclusion process under periodic perturbations [13]. In the present paper, we will explain the numerical method using a simple particle hopping model for pump current problems.

The outline of the present paper is as follows. In section 2 we explain the general scheme for the generating function approach. Section 3 is the main part of the paper and the direct numerical method is presented by way of an example in the pump current problem. In addition, the validity of the proposed method is confirmed by comparison with the Monte Carlo simulations in section 3. Section 4 gives concluding remarks.

2. General formalism for the generating function

We first explain the general formalism for the generating function of the counting statistics. Although the formalism is similar to the one proposed in [5], we here present the general case in which the transition matrix can depend on time.

Denoting the probability of finding the system in state \( n \) by \( p_n(t) \), a master equation for the system is

\[
\frac{\partial}{\partial t} p_n(t) = \sum_m \kappa_{nm}(t) p_m(t),
\]

where \( \{\kappa_{nm}(t)\} \) is a transition matrix. The component \( (n, m) \) of the transition matrix \( \kappa_{nm}(t) \) is the rate of the \( m \to n \) transition, and it can be time dependent.

We here derive the generating function for counting the number of events of a specific transition \( i_A \to j_A \). The generalization to multiple transitions is straightforward.

Firstly, we denote the probability for the system starting in state \( m \) and finishing in state \( n \), with \( N_A \) being the number of \( i_A \to j_A \) transitions during time \( t \), as \( P_{nm}(N_A|t) \). The probability \( P_{nm}(N_A|t) \) is obtained by repeated convolutions of the probability of no transitions, i.e.

\[
P_{nm}(N_A|t) = G'_{nJA}(t) * \underbrace{G'_{iAJ}(t) * \cdots * G'_{iAJ}(t)}_{N_A-1} * \kappa_{jAiA}(t) G'_{iAm}(t),
\]

where \( g_1(t) * g_2(t) \equiv \int_0^t g_1(t - t') g_2(t') \, dt' \) denotes the convolution, and \( G'_{kl}(t) \) is the probability for the system evolving from state \( l \) to state \( k \), provided no \( i_A \to j_A \) transitions occur during time \( t \).

Secondly, the generating function of the probability \( P_{nm}(N_A|t) \) is defined by

\[
f_{nm}(\lambda, t) = \sum_{N_A} \lambda^{N_A} P_{nm}(N_A|t).
\]

One can see that the generating function \( f_{nm}(\lambda, t) \) satisfies the following integral equation:

\[
f_{nm}(\lambda, t) = G'_{nm}(t) + \int_0^t G'_{nJa}(t - t') \lambda \kappa_{jAiA}(t') f_{iAm}(\lambda, t') \, dt'.
\]
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Thirdly, we derive the time-evolution equation for the generating function $f_{nm}(\lambda, t)$. We notice that the probability of no transitions, $G'_{nm}(t)$, obeys

$$\frac{\partial}{\partial t} G'_{nm}(t) = \sum_i \kappa_{ni}(t) G'_{im}(t) - \delta_{n, j_A} \kappa_{j_A i_A}(t) G'_{i_A m}(t), \quad (5)$$

where $\delta_{i, j}$ is the Kronecker delta. Hence, using the differentiation of the convolution,

$$\frac{\partial}{\partial t} \int_0^t g_1(t - t') g_2(t') dt' = g_1(0) g_2(t) + \int_0^t \left( \frac{\partial}{\partial t} g_1(t - t') \right) g_2(t') dt', \quad (6)$$

the time-evolution equation for $f_{nm}(\lambda, t)$ is derived as follows:

$$\frac{\partial}{\partial t} f_{nm}(\lambda, t) = \sum_i \kappa_{ni}(t) f_{im}(\lambda, t) - \delta_{n, j_A} \kappa_{j_A i_A}(t) f_{i_A m}(\lambda, t) + \lambda G'_{n j_A}(0) \kappa_{j_A i_A}(t) f_{i_A m}(\lambda, t)$$

$$+ \int_0^t \left( \frac{\partial}{\partial t} G'_{n j_A}(t - t') \right) \lambda \kappa_{j_A i_A}(t') f_{i_A m}(\lambda, t) dt'$$

$$= \sum_i \kappa_{ni}(t) f_{im}(\lambda, t) - \delta_{n, j_A} (1 - \lambda) \kappa_{j_A i_A}(t) f_{i_A m}(\lambda, t), \quad (7)$$

where we used $G'_{nm}(0) = \delta_{n, m}$. Equation (7) should be solved with the initial conditions $f_{nm}(\lambda, 0) = \delta_{n, m}$.

Finally, we construct the generating function for counting the number of the target $i_A \rightarrow j_A$ transitions, i.e.,

$$F(\lambda, t) = \sum_{N_A=0}^{\infty} \lambda^{N_A} P(N_A|t). \quad (8)$$

Since $f_{nm}(\lambda, t)$ is the generating function with specific initial state $m$ and final state $n$, the generating function with specific final state $n$ is constructed as

$$\phi_n(\lambda, t) = \sum_m f_{nm}(\lambda, t) p_m(0), \quad (9)$$

where $p_m(0)$ is a probability distribution at initial time $t = 0$. Hence the generating function $F(\lambda, t)$ is calculated as

$$F(\lambda, t) = \sum_n \phi_n(t). \quad (10)$$

In addition, the time-evolution equation for the generating function $\phi_n(\lambda, t)$ is given by

$$\frac{\partial}{\partial t} \phi_n(\lambda, t) = \sum_m \frac{\partial}{\partial t} f_{nm}(\lambda, t) p_m(0)$$

$$= \sum_m \left[ \sum_i \kappa_{ni}(t) f_{im}(\lambda, t) - \delta_{n, j_A} (1 - \lambda) \kappa_{j_A i_A}(t) f_{i_A m}(\lambda, t) \right] p_m(0)$$

$$= \sum_i \kappa_{ni}(t) \phi_i(\lambda, t) - \delta_{n, j_A} (1 - \lambda) \kappa_{j_A i_A}(t) \phi_{i_A}(\lambda, t), \quad (11)$$

and these equations should be solved with initial conditions $\phi_n(0) = \sum_m f_{nm}(\lambda, 0) p_m(0) = p_n(0)$.

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3. A direct numerical method for obtaining the moments

In order to explain the new direct numerical method for calculating moments in the counting statistics, we use a simple stochastic model with two states; the discussion is easily extended to general cases with \( N \) states.

The stochastic process with two states has been proposed in [9] in the context of the pump current problem. The system consists of three parts, as shown in figure 1. The container can contain at most one particle. When the container is filled with one particle the particle can escape from the container by jumping into either one of the two particle baths, i.e., the left reservoir \([L]\) or the right one \([R]\). In the pump current problem, the \( k_{\pm 1} \) and \( k_{\pm 2} \) transition rates depend on time, and here we set them as

\[
k_{-1} = k_2 = 1, \quad k_1 = 1 + R \cos(\omega t), \quad k_{-2} = 1 + R \sin(\omega t).
\]

Defining \( p_1 \) and \( p_2 \) as the respective probabilities of the container being empty or filled, the master equation is written as

\[
\frac{\partial}{\partial t} \begin{pmatrix} p_1(t) \\ p_2(t) \end{pmatrix} = \begin{pmatrix} -k_1 - k_{-2} & k_{-1} + k_2 \\ k_1 + k_{-2} & -k_{-1} - k_2 \end{pmatrix} \begin{pmatrix} p_1(t) \\ p_2(t) \end{pmatrix}.
\]

In order to estimate the particle current from the container to the right reservoir \([R]\) we need to count the number of transitions from the container to the right reservoir \([R]\) and the number of transitions from \([R]\) to the container; we should calculate the difference between them. According to section 2, the generating function for the particle current is given by

\[
F(\lambda, t) = \phi_1(\lambda, t) + \phi_2(\lambda, t),
\]

where \( \phi_1(\lambda, t) \) and \( \phi_2(\lambda, t) \) obey the following time-evolution equations:

\[
\frac{\partial}{\partial t} \phi_1(\lambda, t) = (-k_1 - k_{-2})\phi_1(\lambda, t) + (k_{-1} + k_2)\lambda \phi_2(\lambda, t),
\]

\[
\frac{\partial}{\partial t} \phi_2(\lambda, t) = (k_1 + k_{-2} \lambda^{-1})\phi_1(\lambda, t) + (-k_{-1} - k_2)\phi_2(\lambda, t).
\]

Note that the transition from the container to \([R]\) gives positive contributions to the statistics, so we multiply \( k_2 \) by \( \lambda \). In contrast, because the transition from \([R]\) to the container gives negative contributions, \( \lambda^{-1} \) is multiplied by \( k_{-2} \).

If we obtain the explicit solution for the generating function \( \phi_1(\lambda, t) \), all statistical information for the particle current is estimated. However, in general it is difficult to obtain the explicit solution for the generating function. Instead of seeking analytic solutions, we proceed to obtain some moments directly via numerical calculations. To this effect, we need to derive the time-evolution equations of the moments. Firstly, \( \lambda \)
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in (15) and (16) is set to 1:

\[
\frac{\partial}{\partial t} \phi_1|_{\lambda=1} = (-k_1 - k_{-2})\phi_1|_{\lambda=1} + (k_{-1} + k_2)\phi_2|_{\lambda=1},
\]

\[
\frac{\partial}{\partial t} \phi_2|_{\lambda=1} = (k_1 + k_{-2})\phi_1|_{\lambda=1} + (-k_{-1} - k_2)\phi_2|_{\lambda=1},
\]

where we denoted \(\phi_1(\lambda = 1, t)\) as \(\phi_1|_{\lambda=1}\) for simplicity. Because (17) and (18) are exactly the same as the original master equation (13), \(\phi_i|_{\lambda=1}\) is interpreted as the probability in the original master equation, i.e., \(\phi_1|_{\lambda=1} = p_1(t)\) and \(\phi_2|_{\lambda=1} = p_2(t)\). Next, the first derivatives of (15) and (16) with respect to \(\lambda\) are calculated and again \(\lambda\) is set to 1:

\[
\frac{\partial}{\partial t} \left[ \frac{\partial \phi_1}{\partial \lambda} \right]_{\lambda=1} = (-k_1 - k_{-2}) \left[ \frac{\partial \phi_1}{\partial \lambda} \right]_{\lambda=1} + k_2p_2 + (k_{-1} + k_2) \left[ \frac{\partial \phi_2}{\partial \lambda} \right]_{\lambda=1},
\]

\[
\frac{\partial}{\partial t} \left[ \frac{\partial \phi_2}{\partial \lambda} \right]_{\lambda=1} = -k_{-2}p_1 + (k_1 + k_{-2}) \left[ \frac{\partial \phi_1}{\partial \lambda} \right]_{\lambda=1} + (-k_{-1} - k_2) \left[ \frac{\partial \phi_2}{\partial \lambda} \right]_{\lambda=1}.
\]

Hence, the first moment of the particle current is calculated as follows:

\[
\frac{\partial}{\partial t} \langle n \rangle = \frac{\partial}{\partial t} \left[ \frac{\partial \phi_1}{\partial \lambda} \right]_{\lambda=1} + \frac{\partial \phi_2}{\partial \lambda} \right]_{\lambda=1} = k_2p_2 - k_{-2}p_1,
\]

which recovers the well-known result [9].

The second and third ‘factorial’ moments are also estimated as follows:

\[
\frac{\partial}{\partial t} \langle n(n-1) \rangle = \frac{\partial}{\partial t} \left[ \frac{\partial^2 \phi_1}{\partial \lambda^2} \right]_{\lambda=1} + \frac{\partial^2 \phi_2}{\partial \lambda^2} \right]_{\lambda=1} = 2k_2 \left[ \frac{\partial \phi_2}{\partial \lambda} \right]_{\lambda=1} + 2k_{-2}p_1 - 2k_{-2} \left[ \frac{\partial \phi_1}{\partial \lambda} \right]_{\lambda=1},
\]

and

\[
\frac{\partial}{\partial t} \langle n(n-1)(n-2) \rangle = \frac{\partial}{\partial t} \left[ \frac{\partial^3 \phi_1}{\partial \lambda^3} \right]_{\lambda=1} + \frac{\partial^3 \phi_2}{\partial \lambda^3} \right]_{\lambda=1} = 3k_2 \left[ \frac{\partial^2 \phi_2}{\partial \lambda^2} \right]_{\lambda=1} - 6k_{-2}p_1 + 6k_{-2} \left[ \frac{\partial \phi_1}{\partial \lambda} \right]_{\lambda=1} - 3k_{-2} \left[ \frac{\partial^2 \phi_1}{\partial \lambda^2} \right]_{\lambda=1}.
\]

The time-evolution equations for \(\partial^2 \phi_i/\partial \lambda^2\) are easily obtained, in a similar way to (19) and (20). In numerical estimation of the time development of the differential equations, all \(\partial^p \phi_i/\partial \lambda^n\) are set to 0 initially, because \(\phi_i(\lambda, 0) = p_i(0)\) does not depend on \(\lambda\) initially. It is easy to obtain the second and third moments from the above factorial moments.

In order to calculate the \(m\)th moment, we should solve \(m \times 2\) coupled differential equations. Generally, when a stochastic process involves \(N\) states, we need \(m \times N\) coupled differential equations to obtain moments up to \(m\)th order. Hence, without using any Monte Carlo method, we can deterministically calculate the moments for the particle current or the number of specific transitions.

To confirm the validity of the new direct numerical method, we compare results obtained from the new method with those from the Monte Carlo method, i.e., the time-dependent Gillespie algorithm [14]. The parameters are \(R = 0.5\) and \(\omega = 4.0\), and the initial state is \(p_1 = 1\) (hence, \(p_2 = 0\)); the container is empty at the initial time. In

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one data set, $10^5$ Monte Carlo trajectories were used to estimate moments of the particle current. We repeated the Monte Carlo calculations, and collected 100 data sets. The error bars in figure 2 correspond to the standard deviation in the 100 data sets. Although we can calculate moments at arbitrary time in the Monte Carlo calculations, we plotted only some points for reference. The results from the new method and those from the Monte Carlo method agree completely.

4. Concluding remarks

In the present paper, a new numerical method for estimating moments for current statistics was proposed. The proposed method needs only time integrations of a system of coupled differential equations, so the moments are estimated deterministically without the aid of Monte Carlo simulations. By way of an example, we explained the proposed method using a simple two-state model. It is easy to apply this method to an arbitrary stochastic process with a finite state space, although the algebraic manipulations become somewhat involved if the state space becomes too large.

In studies of a nonequilibrium current or nonequilibrium properties, it would be valuable to obtain detailed information about the statistics of the current. If one can obtain analytical solutions for the generating function, all statistical information, including the probability distribution for the current, is calculated from the solutions. However, it is difficult in general to treat a case with a complicated time-dependent transition matrix. On the other hand, the proposed numerical method is applicable for arbitrary time dependence, and we believe that the proposed method will prove both important
A direct numerical method for obtaining the counting statistics for stochastic processes and useful for cases in which an analytical solution of the nonequilibrium current is out of reach.

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