INVITED PAPER *Special Section on Progress in Information Network Science*

Basics of Counting Statistics

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SUMMARY In this paper, we briefly review the scheme of counting statistics, in which a probability of the number of monitored or target transitions in a Markov jump process is evaluated. It is generally easy to construct a master equation for the Markov jump process, and the counting statistics enables us to straightforwardly obtain basic equations of the counting statistics from the master equation; the basic equation is used to calculate the cumulant generating function of the probability of the number of target transitions. For stationary cases, the probability is evaluated from the eigenvalue analysis. As for the nonstationary cases, we review a numerical integration scheme to calculate the statistics of the number of transitions.

key words: *stochasticity, numerical method, generating function approach, path-integral approach*

1. Introduction

Stochasticity has become one of the key concepts in various research fields, ranging from engineering fields to physical or biological fields. There are many sources of uncertainty in various phenomena, and various studies have been performed in order to deal with the stochastic behaviour caused by the uncertainty.

Of course, if we consider large-scale phenomena, it is sometimes possible to neglect such stochasticity or effects of 'noise'. A typical example is a chemical reaction system; chemical reactions occur in a probabilistic way in a microscopic point of view, but when we consider a test-tube experiment the stochastic behavior can be neglected and the rate equation approach is employed in general. (For the general theory of the stochasticity, see Ref. [1], for example.) There are many analysis focusing on only the average behaviors; for example, the flux balance analysis is one of the important research topics in large-scale biochemical networks, and only the average flux is considered [2]. However, recent development of experimental techniques enables us to investigate effects of stochasticity or fluctuation, and it has been revealed that the stochasticity is sometimes important and necessary for living matters [3].

In order to deal with such stochastic behaviors, many analytical and theoretical methods have been developed [1], especially in physics and chemical biology. One of the recent developments is the *counting statistics*. It is also called the *full counting statistics*, because all stochasticity or fluctuations are considered and evaluated in the scheme. That is, not only the average, but also higher order moments or cumulants are evaluated in the scheme. (Although the counting statistics is also used in quantum systems [4], we only treat classical systems in the present paper.)

The main aim of the present paper is to briefly review the scheme of the counting statistics. When we consider a Markov jump process, the counting statistics enables us to evaluate all statistics for the number of *monitored* or *target* transitions. One of the remarkable features is that there is a straightforward way to calculate the statistics from the master equation which describes state changes in the Markov jump process. Although such evaluations are deeply related to the renewal theory [5] as discussed in Ref. [6], the counting statistics gives us a simple way for the calculation starting from the master equation. It is generally easy to construct the master equation, and hence the scheme of the counting statistics will become a powerful tool to evaluate the statistics of transitions. The counting statistics has been mainly used in order to investigate small systems; we will explain one example in Sect. 2. Applications of the counting statistics to large scale networks are future works, and it will be needed to develop practical approximation methods or effective calculation schemes in order to employ the counting statistics for studies of networks. We hope that the brief review will motivate and help such future works.

The outline of the present paper is as follows. In Sect. 2, the problem settings and a stochastic model related to networks are explained. A simple way to investigate such stochastic model is a direct computer simulation, and hence a brief review of Monte Carlo simulations for the stochastic model is shown in Sect. 3. Although the Monte Carlo simulations are helpful and useful to investigate the statistics of the number of target transitions, sometimes long computational times are needed to perform the Monte Carlo simulations. Hence, the scheme of the counting statistics is needed; Sect. 4 gives a brief review of the counting statistics. For stationary cases, in which all transition rates are time-independent, it is sometimes easy to obtain analytic solutions for the statistics in stationary states. In contrast, when we consider non-stationary cases, it is in general impossible to obtain such analytic solutions. For the time-dependent cases, a direct numerical method has been proposed [7], and the numerical method is also reviewed in Sect. 4. Section 5 gives some concluding remarks.

Manuscript received March 7, 2013.
Manuscript revised June 13, 2013.

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DOI: 10.1587/transcom.E96.B.2733

2. Problem Settings

In this section, we explain problem settings in a manner that it helps to imagine applications for network sciences.

Figure 1 shows a network model. The network model consists of three components; nodes, edges, and particles on nodes. We here assume each node can contain at most one particle. Hence, there are only two states for a node, i.e., 'empty' state or 'filled' state. Each node can emit the particle to neighbor nodes connected to the node. When a node has a particle, the node cannot receive a particle from the neighbor nodes, as shown in Fig. 1. The particle hopping occurs probabilistically. The problem here is to investigate the particle hopping or particle flow on the network.

In order to simplify the problem, we consider only the node enclosed by the dashed circle in Fig. 1. The node is connected to two nodes, i.e., the left side and the right side. In addition, we assume that the outside of the dashed circle is filled with a sufficient number of particles, and hence when the node is empty, a particle can hop into the node from the left or right sides independently of the states of the left and right sides. Moreover, there is an assumption that the outside of the dashed circle can always receive a particle from the node. These assumptions mean that we assume two particle baths or reservoirs connected to the node. While the assumptions may seem to be crude or unnatural because we neglect the network structure, the following discussions can be extended to network structures formally. In addition, the particle baths can simply be considered as the outside of the network.

In order to construct the mathematical model for the problem settings, it is needed to define transition rates (for details of the Markov jump process, see [8] for example). There are four transition rates, as depicted in Fig. 1; when the node is empty a particle hopping from the left side occurs with rate $k_{-\mathrm{L}}(t)$; there is a particle hopping from the filled node to the left side with rate $k_{\mathrm{L}}(t)$, and so on. Here, the minus sign in the subscript in $k_{-\mathrm{L}}$ or $k_{-\mathrm{R}}$ means the fact that a particle number of the left or right side decreases due to the particle hopping. Note that the particle hopping depends on the state of the node; when the node is filled, there is no particle hopping from the left or right side. In addition, we assume that all transition rates are time-dependent.

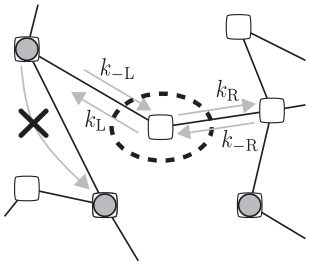

Fig. 1 A stochastic particle transport on a network. Each node can contain at most one particle, and the particle hopping from a filled node to another filled node is forbidden, as depicted. We here focus only on the behaviour of the node enclosed by the dashed circle, and we assume that the outside of the dashed circle can always receive and emit a particle.

We here consider the following question: Is the state of the node 'empty' at time t? Of course, the model is a stochastic one, so it is impossible to answer this question. However, it is still possible to answer the probability with which the node is empty at time t. Such probabilities are calculated by using a master equation, and the master equation is easily constructed from the transition rates, as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} p_{\mathrm{e}}(t) \\ p_{\mathrm{f}}(t) \end{pmatrix} = \begin{pmatrix} -k_{-\mathrm{L}}(t) - k_{-\mathrm{R}}(t) & k_{\mathrm{L}}(t) + k_{\mathrm{R}}(t) \\ k_{-\mathrm{L}}(t) + k_{-\mathrm{R}}(t) & -k_{\mathrm{L}}(t) - k_{\mathrm{R}}(t) \end{pmatrix}\begin{pmatrix} p_{\mathrm{e}}(t) \\ p_{\mathrm{f}}(t) \end{pmatrix}, \tag{1}$$

where p_{e} and p_{f} are the probabilities with which the state of the node is 'empty' and 'filled', respectively.

The next question is: What is the average of the number of transitions from the node to the right side? The answer is as follows. At time t, the node is filled with probability $p_{\mathrm{f}}(t)$, and there is a particle hopping from the node to the right side with rate $k_{\mathrm{R}}(t)$. Hence, we expect $k_{\mathrm{R}}(t)p_{\mathrm{f}}(t)$ times particle hopping at time t in average. The average of the number of transitions from the node to the right side is therefore given as the integral of the instantaneous hopping numbers, i.e., $\int k_{\mathrm{R}}(t)p_{\mathrm{f}}(t)\mathrm{d}t$.

What is the average *net* flow from the node to the right side? In order to consider it, we define a particle hopping from the node to the right side as $+1$ contribution, and a particle hopping from the right side to the node as -1 contribution for the flow. Hence, the instantaneous hopping numbers are given by $k_{\mathrm{R}}(t)p_{\mathrm{f}}(t) - k_{-\mathrm{R}}(t)p_{\mathrm{e}}(t)$, and the average flow is calculated from $\int (k_{\mathrm{R}}(t)p_{\mathrm{f}}(t) - k_{-\mathrm{R}}(t)p_{\mathrm{e}}(t))\mathrm{d}t$.

How about the variance of the flow? Different from the average flow, in general it is impossible to evaluate the variance of the flow from the solutions of the master equation, $p_{\mathrm{e}}(t)$ and $p_{\mathrm{f}}(t)$. How about higher order moments or cumulants? It is expected that such higher order moments or cumulants will help to characterize the particle flows. In addition, when some of the transition rates are unknown, observations of the higher order moments will be important for parameter estimation problems. Hence, it is needed to evaluate such statistics from the stochastic model.

3. Monte Carlo Simulations

A simple way to evaluate the statistics from the stochastic model is to perform Monte Carlo simulations. Using the Monte Carlo simulations, many sample trajectories are created, and they are used to evaluate the statistics.

We here briefly explain one of the famous Monte Carlo method, which is called sometimes Gillespie algorithm [9]. For notational simplicity, four transitions are abbreviated as follows:

R1. Left $\to$ Node (at rate $k_{-\mathrm{L}}$).
R2. Node $\to$ Left (at rate k_{L}).
R3. Right $\to$ Node (at rate $k_{-\mathrm{R}}$).

R4. Node → Right (at rate k_R).

Reactions R1 and R3 occur only when the node is 'empty', and after the reactions, the state of the node is changed to 'filled'. In contrast, the node in the 'filled' state can cause reaction R2 or R4 with the state change from 'filled' to 'empty'. Firstly, we explain a simulation method for a *time-independent* case; all transition rates are time-independent.

Monte Carlo algorithm for the stochastic model

1. Set $p_e(0)$. The initial state is chosen as 'empty' according to the probability $p_e(0)$. (Hence, the state is selected as 'filled' with the probability $p_f(0) = 1 - p_e(0)$). Set $t = 0$.
2. Generate a uniform random number r from the interval $(0, 1)$.
3. Set a time interval Δ as follows.
   - If the state is 'empty', $\Delta = \ln(1/r)/(k_{-L} + k_{-R})$.
   - If the state is 'filled', $\Delta = \ln(1/r)/(k_L + k_R)$.

   Note that the above time interval is equivalent to drawing an exponential random variable with parameter $(k_{-L} + k_{-R})$ and $(k_L + k_R)$, respectively.
4. Select a reaction, as follows.
   - If the state is 'empty', choose reaction R1 (or R3) with the probability $k_{-L}/(k_{-L}+k_{-R})$ (or $k_{-R}/(k_{-L}+k_{-R})$).
   - If the state is 'filled', choose reaction R2 (or R4) with the probability $k_L/(k_L+k_R)$ (or $k_R/(k_L+k_R)$).
5. Put $t \to t + \Delta$.
6. Change the state ('empty' → 'filled' or 'filled' → 'empty').
7. Return to step 2 until the simulation is ended.

When the transition rates, k_L, k_{-L}, k_R, and k_{-R}, are time-dependent, the steps 3 and 4 in the above algorithm are changed as follows [10].

3'. Set a time interval Δ to satisfy the following equations.
   - If the state if 'empty',

$$\int_t^{t+\Delta} (k_{-R}(\tau) + k_{-L}(\tau))\,d\tau = \ln\left(\frac{1}{r}\right).$$

   - If the state if 'filled',

$$\int_t^{t+\Delta} (k_R(\tau) + k_L(\tau))\,d\tau = \ln\left(\frac{1}{r}\right).$$

4'. Select a reaction, as follows.
   - If the state is 'empty', choose reaction R1 (or R3) with the probability

$$\frac{k_{-L}(t+\Delta)}{k_{-L}(t+\Delta) + k_{-R}(t+\Delta)} \left(\text{or} \quad \frac{k_{-R}(t+\Delta)}{k_{-L}(t+\Delta) + k_{-R}(t+\Delta)}\right).$$

   - if the state is 'filled', choose reaction R2 (or R4) with the probability

$$\frac{k_L(t+\Delta)}{k_L(t+\Delta) + k_R(t+\Delta)} \left(\text{or} \quad \frac{k_R(t+\Delta)}{k_L(t+\Delta) + k_R(t+\Delta)}\right).$$

In Ref. [10], more efficient algorithm is explained.

Using the above algorithm, we can generate many sample trajectories, and the number of specific transitions is counted from the sample trajectories. It is therefore possible to construct the probability distribution of the number of specific transitions. In addition, higher order moments or cumulants are also easily evaluated. However, many sample trajectories are needed in order to obtain precise estimations of the statistics, and the Monte Carlo algorithm takes a long computational time in general.

4. Counting Statistics

In this section, we briefly review the consequences of the scheme of the counting statistics, using some specific examples. Detailed information for the counting statistics is available in Refs. [6] and [11], for example.

4.1 Number of Transitions from the Node to the Right Side in Steady-State

Firstly, we calculate the statistics of the number of transitions from the node to the right side. In addition, only the time-independent and steady-state is considered.

In order to evaluate the statistics of the number of transitions, it is a common way to construct the generating function. We define the probability $P(N|T)$ with which there are N target transitions during time interval $[0, T]$. The generating function for $P(N|T)$ is therefore defined as

$$F(\lambda, T) \equiv \sum_{N=0}^{\infty} P(N|T)\lambda^N. \tag{2}$$

Note that all statistics can be calculated from the generating functions. For example, the average of N, $\langle N\rangle$, is given as $\partial F(\lambda, T)/\partial\lambda|_{\lambda=1}$. The second factorial moment is given by $\langle N(N-1)\rangle = \partial^2 F(\lambda, T)/\partial\lambda^2|_{\lambda=1}$, and so on. However, we do not know the probability $P(N|T)$, which is needed to define the generating function $F(\lambda, T)$. The consequence of the counting statistics is that the generating function $F(\lambda, T)$ is given as the following simple summation;

$$F(\lambda, T) = \phi_e(\lambda, T) + \phi_f(\lambda, T), \tag{3}$$

where $\phi_e(\lambda, T)$ and $\phi_f(\lambda, T)$ are the solutions at time T of the following time-evolution equations;

$$\frac{d}{dt}\begin{pmatrix}\phi_e(\lambda,t)\\ \phi_f(\lambda,t)\end{pmatrix} = \begin{pmatrix}-k_{-L} - k_{-R} & k_L + \lambda k_R\\ k_{-L} + k_{-R} & -k_L - k_R\end{pmatrix}\begin{pmatrix}\phi_e(\lambda,t)\\ \phi_f(\lambda,t)\end{pmatrix}. \tag{4}$$

As the initial values, we set $\phi_e(\lambda, 0) = p_e(0)$ and $\phi_f(\lambda, 0) =$

$p_{\rm f}(0)$. The derivation of the above equations in more general settings is briefly explained in the Appendix A in two ways; in Sect. A.1, we show a conventional one based on the generating function approach [11], and Sect. A.2 gives more intuitive one based on the path integral approach. Although the derivation is a little complicated, the final consequence is simple; Eq. (4) is very similar to the original master Eq. (1). Differences are as follows: we use $\phi_{\rm e}(\lambda, t)$ and $\phi_{\rm f}(\lambda, t)$ instead of $p_{\rm e}(t)$ and $p_{\rm f}(t)$; we want to count the number of "node → right" transition, and the new variable λ is multiplied to $k_{\rm R}$, which is related to the target transition. Note that $k_{\rm R}$ in the diagonal elements of the 'transition' matrix in Eq. (1) does not changed. Only the off-diagonal elements are modified.

For the time-independent transition rates, we can calculate the analytic form of the generating function in the steady state, in which the left-hand-side in Eq. (4) is equal to zero. The eigenvalue analysis will help such analysis. Moreover, the probability distribution has been also derived for a similar stochastic model [12], and we employ the result as follows:

$$P(N|T) = \left(\frac{(1-\gamma^2)\tilde{T}}{2\gamma}\right)^N \frac{e^{-\tilde{T}}}{N!\sqrt{8\gamma\tilde{T}/\pi}} \times \left\{2\gamma(N+\tilde{T})I_{N-1/2}(\gamma\tilde{T}) + (1+\gamma^2)\tilde{T}I_{N+1/2}(\gamma\tilde{T})\right\}, \quad (5)$$

where $\tilde{T} = (k_{\rm L} + k_{-\rm L} + k_{\rm R} + k_{-\rm R})T/2$, $\gamma^2 = 1 - 4k_{\rm R}(k_{-\rm L} + k_{-\rm R})/(k_{\rm L} + k_{-\rm L} + k_{\rm R} + k_{-\rm R})^2$, and $I_n(z)$ are modified Bessel functions of the first kind.

4.2 Flow from the Node to the Right Side in Non-Stationary Cases

As a next example, we consider the net flow from the node to the right side. As explained in Sect. 2, the net flow is calculated by subtracting the number of hopping "right → node" from that of "node → right". In addition, in order to treat more general settings, all transition rates are assumed to be time-dependent. Although perturbation analysis gives the approximate analytic solutions for some special cases [13], it is generally impossible to obtain the analytic solutions for the generating function in the time-dependent cases. Hence, we here employ a numerical scheme to evaluate the statistics, i.e., factorial moments.

As briefly discussed in Appendix A.2, such *multiple* target transitions can be also easily treated in the scheme of the counting statistics. For the flow case, we must consider that the *net* number of transitions becomes negative; if there are many "right → node" hopping, the net number may become negative. As a result, the probability with which there are N net transitions from the node to the right side, $P(N|T)$, during time interval $[0, t]$ is defined and calculated as follows:

$$F(\lambda, T) \equiv \sum_{N=-\infty}^{\infty} P(N|T)\lambda^N = \phi_{\rm e}(\lambda, T) + \phi_{\rm f}(\lambda, T). \quad (6)$$

In addition, the following equation is used to obtain the generating function:

$$\frac{\partial}{\partial t}\begin{pmatrix}\phi_{\rm e}(\lambda,t)\\ \phi_{\rm f}(\lambda,t)\end{pmatrix} = \begin{pmatrix} -k_{-\rm L}(t) - k_{-\rm R}(t) & k_{\rm L}(t) + \lambda k_{\rm R}(t) \\ k_{-\rm L}(t) + \lambda^{-1}k_{-\rm R}(t) & -k_{\rm L}(t) - k_{\rm R}(t)\end{pmatrix}\begin{pmatrix}\phi_{\rm e}(\lambda,t)\\ \phi_{\rm f}(\lambda,t)\end{pmatrix}. \quad (7)$$

Note that the new variable λ is multiplied to the transition rate $k_{\rm R}(t)$ which is related to the positive contribution, i.e., hopping "node → right". In contrast, its inverse, λ^{-1}, is used for the transition rate $k_{-\rm R}$, which is related to "right → node" hopping, i.e., the negative contribution. Only these modifications are enough to evaluate the generating function.

The question considered here is as follows: Is it possible to evaluate *instantaneous* (factorial) moments for the time-dependent case? Once the instantaneous (factorial) moments are evaluated, the (factorial) moments during time interval $[0, T]$ can be obtained from the numerical integrations. The intuitive discussion in Sect. 2 gives the instantaneous *average flow* from the solution of the master equation. In the following, we show that we can recover the result for the average flow by using the counting statistics, and furthermore, the higher-order factorial moments are also easily evaluated from the numerical integrations [7].

When we set $\lambda = 1$ in Eq. (7), the following equations are derived:

$$\frac{\partial}{\partial t}\phi_{\rm e}(\lambda,t)|_{\lambda=1} = (-k_{-\rm L}(t) - k_{-\rm R}(t))\phi_{\rm e}(\lambda,t)|_{\lambda=1} + (k_{\rm L}(t) + k_{\rm R}(t))\phi_{\rm f}(\lambda,t)|_{\lambda=1}, \quad (8)$$

$$\frac{\partial}{\partial t}\phi_{\rm f}(\lambda,t)|_{\lambda=1} = (k_{-\rm L}(t) + k_{-\rm R}(t))\phi_{\rm e}(\lambda,t)|_{\lambda=1} + (-k_{\rm L}(t) - k_{\rm R}(t))\phi_{\rm f}(\lambda,t)|_{\lambda=1}. \quad (9)$$

Note that Eqs. (8) and (9) are quite identical to the original master Eq. (1). Hence, we can interpret $\phi_{\rm e}(\lambda, t)|_{\lambda=1}$ and $\phi_{\rm f}(\lambda, t)|_{\lambda=1}$ as $p_{\rm e}(t)$ and $p_{\rm f}(t)$, respectively.

Next, the first derivatives of Eq. (7) with respect to λ are calculated and again λ is set to 1. We therefore obtain the following equations:

$$\frac{\partial}{\partial t}\left.\frac{\partial\phi_{\rm e}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1} = (-k_{-\rm L}(t) - k_{-\rm R}(t))\left.\frac{\partial\phi_{\rm e}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1} + k_{\rm R}(t)p_{\rm f}(t) + (k_{\rm L}(t) + k_{\rm R}(t))\left.\frac{\partial\phi_{\rm f}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1}, \quad (10)$$

$$\frac{\partial}{\partial t}\left.\frac{\partial\phi_{\rm f}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1} = -k_{-\rm R}(t)p_{\rm e}(t) + (k_{-\rm L}(t) + k_{-\rm R}(t))\left.\frac{\partial\phi_{\rm e}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1} + (-k_{\rm L}(t) - k_{\rm R}(t))\left.\frac{\partial\phi_{\rm f}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1}. \quad (11)$$

The above four equations are enough to evaluate the moments up to the second-order. The instantaneous average flow, $\partial\langle N(t)\rangle/\partial t$, is calculated by taking the first derivative of the generating function $F(\lambda, t)$; the first moment of the net flow is calculated as follows:

$$\frac{\partial}{\partial t}\langle N(t)\rangle = \frac{\partial}{\partial t}\left[\left.\frac{\partial\phi_{\rm e}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1} + \left.\frac{\partial\phi_{\rm f}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1}\right] = k_{\rm R}(t)p_{\rm f}(t) - k_{-\rm R}(t)p_{\rm e}(t), \tag{12}$$

where Eqs. (10) and (11) were used, and the identifications ($\phi_{\rm e}(\lambda,t)|_{\lambda=1} = p_{\rm e}(t)$ and $\phi_{\rm f}(\lambda,t)|_{\lambda=1} = p_{\rm f}(t)$) were employed. Hence, the intuitive result discussed in Sect. 2 is adequately recovered.

Furthermore, it is also possible to evaluate the second factorial moment as follows.

$$\begin{aligned}\frac{\partial}{\partial t}&\langle N(t)\,(N(t)-1)\rangle \\ &= \frac{\partial}{\partial t}\left[\left.\frac{\partial^2\phi_{\rm e}(\lambda,t)}{\partial\lambda^2}\right|_{\lambda=1} + \left.\frac{\partial^2\phi_{\rm f}(\lambda,t)}{\partial\lambda^2}\right|_{\lambda=1}\right] \\ &= 2k_{\rm R}(t)\left.\frac{\partial\phi_{\rm f}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1} + 2k_{-\rm R}(t)p_{\rm e}(t) \\ &\quad - 2k_{-\rm R}\left.\frac{\partial\phi_{\rm e}(\lambda,t)}{\partial\lambda}\right|_{\lambda=1}.\end{aligned} \tag{13}$$

Higher-order moments can be evaluated in a similar way, although we need more equations similar to Eqs. (10) and (11). Using this scheme, it is possible to evaluate the statistics (factorial moments) at least numerically. Of course, the above numerical integration scheme is an exact one except for numerical errors, and the numerical integration is more rapid than the Monte Carlo methods in general.

We here give some comments for the numerical integrations. As for the initial settings in the numerical integrations, we use the following ones; $\partial\phi_{\rm e}(\lambda,0)|_{\lambda=1} = p_{\rm e}(0)$ and $\partial\phi_{\rm f}(\lambda,0)|_{\lambda=1} = p_{\rm f}(0)$; the higher-order derivatives of $\phi_{\rm e}$ and $\phi_{\rm f}$ are set to 0 initially.

As a numerical example, we consider the following settings: $k_{-\rm L}(t) = t$ and $k_{\rm L}(t) = k_{\rm R}(t) = k_{-\rm R}(t) = 1.0$. As the initial condition, $p_{\rm e}(0) = 1$ is used. The 1st moment is evaluated by the direct numerical integration of Eq. (12), and the 2nd moment is calculated from the second 'factorial' moment (Eq. (13)) and the first moment. The results are shown in Fig. 2. The Monte Carlo results are also shown; 10^3 Monte Carlo trajectories were used to estimate 1st and 2nd moments, and the Monte Carlo simulations are repeated 100 times; the error bars in Fig. 2 correspond to the standard deviation in the 100 data sets. We note that the direct numerical evaluation is rapid, and it gives accurate results.

5. Concluding Remarks

In the present paper, the brief review of the scheme of the counting statistics was explained. For some specific cases, it is possible to calculate all statistics of the number of target transitions analytically. For the time-dependent cases, the numerical scheme enables us to evaluate the factorial moments without using the Monte Carlo simulations.

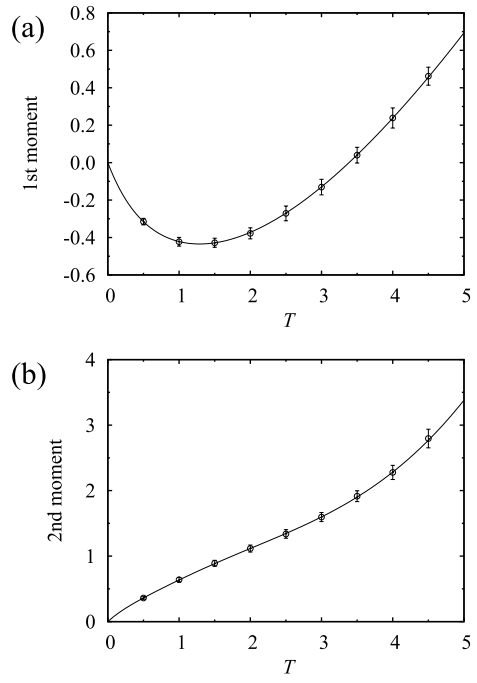

Fig. 2 Moments obtained by the direct numerical method (solid lines) and the Monte Carlo method (circles with error bars). (a) First moment. (b) Second moment. In the example, we set $k_{-\rm L}(t) = t$ and $k_{\rm L}(t) = k_{\rm R}(t) = k_{-\rm R}(t) = 1.0$; $p_{\rm e}(0) = 1$.

As written in Sect. 1, only the basic concepts and methods were shown here. It is possible to calculate more detailed information for the target transitions [6]. In addition, there is a work which would be directly related to a context of network science [14]. It has also been clarified that interesting mathematical structures are behind the counting statistics for time-dependent cases [7], [15]–[18]. Furthermore, the scheme of the counting statistics can be applied in order to investigate other quantities related to the transitions; for example, the entropy production has been studied in the scheme of the counting statistics in Ref. [20]. We hope that the applications of the counting statistics will open up a new horizon for network sciences.

Acknowledgements

This work was supported in part by grant-in-aid for scientific research (Grant No. 25870339) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan.

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Appendix A: Derivation of the 'basic' Equation in the Counting Statistics

For reader's convenience, we here briefly explain the derivation of the 'basic' equation, like Eq. (4), for the counting statistics. The conventional derivation is based on the generating function approach. In Sect. A.1, we summarize the derivation based on Ref. [11], in which only a case with a single target transition is treated. One may consider that it would be difficult and complicated to extend the derivation to cases with multiple target transitions. Hence, in Sect. A.2, an intuitive derivation based on the path-integral approach is discussed. As far as we know, it is rare to explain the path-integral approach, and the derivation will help the reader's understandings for the counting statistics. In addition, it has been shown recently that such derivation is deeply related to the algebraic probability theory [21].

A.1 Generating Function Approach

Different from the two-state model in Sect. 2, we here consider a general case, in which there are many states. Let $p_n(t)$ be the probability of finding the system in state n at time t. Then, a master equation for the system is written as

$$\frac{\mathrm{d}}{\mathrm{d}t}p_n(t) = \sum_m K_{nm}(t)p_m(t), \tag{A·1}$$

where $\{K_{nm}(t)\}$ is a transition matrix. The component of the transition matrix, $K_{nm}(t)$, is the transition rate $m \to n$.

We here focus on a specific target transition $i_\mathrm{A} \to j_\mathrm{A}$, and derive the time-evolution equation for the generating function for counting the number of events.

Firstly, let $P_{nm}(N|T)$ be the probability with which the system starts in state m and finishes in state n with N being the number of transitions $i_\mathrm{A} \to j_\mathrm{A}$ during time interval $[0, T]$. It is clear that the following repeated convolutions gives $P_{nm}(N|T)$:

$$\begin{aligned} &P_{nm}(N|T) \\ &= G'_{nj_\mathrm{A}}(T) \\ &\quad * \underbrace{K_{j_\mathrm{A}i_\mathrm{A}}(T)G'_{i_\mathrm{A}j_\mathrm{A}}(T) * \cdots * K_{j_\mathrm{A}i_\mathrm{A}}(T)G'_{i_\mathrm{A}j_\mathrm{A}}(T)}_{N-1} \\ &\quad * K_{j_\mathrm{A}i_\mathrm{A}}(T)G'_{i_\mathrm{A}m}(T), \end{aligned} \tag{A·2}$$

where $g_1(t) * g_2(t) \equiv \int_0^t g_1(t-t')g_2(t')\mathrm{d}t'$ denotes the convolution, and $G'_{kl}(t)$ is the probability with which the system evolves from state l to state k, provided no $i_\mathrm{A} \to j_\mathrm{A}$ transitions occur during time interval $[0, t]$.

Secondly, the generating function of the probability $P_{nm}(N|T)$ is defined by

$$f_{nm}(\lambda, T) = \sum_{N=0}^{\infty} \lambda^N P_{nm}(N|T), \tag{A·3}$$

which satisfies the following integral equation

$$\begin{aligned} &f_{nm}(\lambda, T) \\ &= G'_{nm}(T) + \int_0^T G'_{nj_\mathrm{A}}(T-t')\lambda K_{j_\mathrm{A}i_\mathrm{A}}(t')f_{i_\mathrm{A}m}(\lambda, t')\mathrm{d}t', \end{aligned} \tag{A·4}$$

where we used Eq. (A·2) and the fact $\sum_{N=0}^{\infty}\lambda^N = 1 + \lambda\sum_{N=0}^{\infty}\lambda^N$.

Thirdly, we derive the time-evolution equation for the generating function $f_{nm}(\lambda, T)$. Notice that the probability of no transitions, $G'_{nm}(t)$, obeys

$$\frac{\mathrm{d}}{\mathrm{d}t}G'_{nm}(t) = \sum_i K_{ni}(t)G'_{im}(t) - \delta_{n,j_\mathrm{A}}K_{j_\mathrm{A}i_\mathrm{A}}(t)G'_{i_\mathrm{A}m}(t), \tag{A·5}$$

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

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

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

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}f_{nm}(\lambda,t) &= \sum_i K_{ni}(t)G'_{im}(t) - \delta_{n,j_\mathrm{A}}K_{j_\mathrm{A}i_\mathrm{A}}(t)G'_{i_\mathrm{A}m}(t) \\ &\quad + \lambda G'_{nj_\mathrm{A}}(0)K_{j_\mathrm{A}i_\mathrm{A}}(t)f_{i_\mathrm{A}m}(\lambda,t) \\ &\quad + \int_0^t \left(\frac{\partial}{\partial t}G'_{nj_\mathrm{A}}(t-t')\right)\lambda K_{j_\mathrm{A}i_\mathrm{A}}(t')f_{i_\mathrm{A}m}(\lambda,t')\mathrm{d}t' \\ &= \sum_i K_{ni}(t)f_{im}(\lambda,t) \\ &\quad - \delta_{n,j_\mathrm{A}}(1-\lambda)K_{j_\mathrm{A}i_\mathrm{A}}(t)f_{i_\mathrm{A}m}(\lambda,t), \end{aligned} \quad (\mathrm{A}\cdot 7)$$

where we used Eq. (A· 5) and $G'_{nm}(0) = \delta_{n,m}$. Equation (A· 7) should be solved with the initial conditions $f_{nm}(\lambda, 0) = \delta_{n,m}$.

Finally, we construct the generating function $F(\lambda, T)$ as follows. 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

$$\phi_n(\lambda, T) = \sum_m f_{nm}(\lambda, T)p_m(0), \quad (\mathrm{A}\cdot 8)$$

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

$$F(\lambda, T) = \sum_n \phi_n(\lambda, T). \quad (\mathrm{A}\cdot 9)$$

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

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\phi_n(\lambda,t) &= \sum_m \frac{\partial}{\partial t}f_{nm}(\lambda,t)p_m(0) \\ &= \sum_m \Big[\sum_i K_{ni}(t)f_{im}(\lambda,t) \\ &\qquad - \delta_{n,j_\mathrm{A}}(1-\lambda)K_{j_\mathrm{A}i_\mathrm{A}}(t)f_{i_\mathrm{A}m}(\lambda,t)\Big]p_m(0) \\ &= \sum_i K_{ni}(t)\phi_i(\lambda,t) - \delta_{n,j_\mathrm{A}}(1-\lambda)K_{j_\mathrm{A}i_\mathrm{A}}(t)\phi_{i_\mathrm{A}}(\lambda,t). \end{aligned} \quad (\mathrm{A}\cdot 10)$$

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

A.2 Path-Integral Approach

Introducing the following state vector

$$|p(t)\rangle \equiv \begin{pmatrix} p_1(t) & p_2(t) & \cdots & p_S(t)\end{pmatrix}^\mathrm{T}, \quad (\mathrm{A}\cdot 11)$$

where S is the number of states, the master equation is rewritten as the simple form:

$$\frac{\mathrm{d}}{\mathrm{d}t}|p(t)\rangle = K(t)|p(t)\rangle, \quad (\mathrm{A}\cdot 12)$$

where $K(t)$ is the transition matrix whose components are the transition rates. Note that due to the basic property of the transition matrix, we have

$$K_{ii}(\tau) = -\sum_{j\neq i} K_{ji}(\tau). \quad (\mathrm{A}\cdot 13)$$

(See Eq. (1), for example.)

The state vector $|p(t)\rangle$ at time T is formally written as

$$|p(T)\rangle = \exp\left(\int_0^T K(t)\mathrm{d}t\right)|p(0)\rangle. \quad (\mathrm{A}\cdot 14)$$

Here, we introduce a time-discretization: $\Delta t = T/M$ and $t_j = j\Delta t$ for $j = 1, 2, \ldots, M$. Note that $t_M = T$. Using small Δt, we have

$$|p(t)\rangle \simeq \mathrm{e}^{K(t_M)\Delta t}\mathrm{e}^{K(t_{N-1})\Delta t}\cdots\mathrm{e}^{K(t_0)\Delta t}|p(0)\rangle. \quad (\mathrm{A}\cdot 15)$$

Next, we expand each time-evolution operator $\exp(K(\tau))\Delta t$ at time τ:

$$\begin{aligned}&\mathrm{e}^{K(\tau)\Delta t} \\ &\simeq \mathbf{1} + K(\tau)\Delta t \\ &= \left(\mathbf{1} + \Delta t\sum_i K_{ii}(\tau)T_{ii}\right) + \Delta t\sum_{i,j(i\neq j)} K_{ij}(\tau)T_{ij}, \end{aligned} \quad (\mathrm{A}\cdot 16)$$

where $\mathbf{1}$ is the unit matrix, and T_{ij} is an operator related to the transition from state i to state j; T_{ij} is a $S \times S$ matrix whose components are zero except for the ij component, i.e., $K(\tau) = \sum_{i,j} K_{ij}(\tau)T_{ij}$.

From the expansion in Eq. (A· 16), the following probabilistic interpretation is possible; the transition $i \to j$ (i.e., T_{ij}) occurs with probability $\Delta t\, K_{ij}(\tau)$, and the first term in Eq. (A· 16) corresponds to a case in which no transition occurs. In addition, Eq. (A· 13) guarantees the probability conservation law; the summation of the probabilities for the occurrences of transitions and that of no-transitions is equal to one.

The aim of the counting statistics is to count the number of the target transitions. From the definition of the generating function $F(\lambda, t)$ in Eq. (2), one can see that the power index of λ in Eq. (2) corresponds to the number of target transitions. In the path-integral approach, the target transition $i_\mathrm{A} \to j_\mathrm{A}$ corresponds to the term $\Delta t\, K_{i_\mathrm{A}j_\mathrm{A}}T_{i_\mathrm{A}j_\mathrm{A}}$; this fact corresponds to the multiplication of λ to the term $\Delta t\, K_{i_\mathrm{A}j_\mathrm{A}}T_{i_\mathrm{A}j_\mathrm{A}}$. As a result, the following replacement for the 'off-diagonal' part of the transition matrix $K(t)$ is needed:

$$K_{i_\mathrm{A}j_\mathrm{A}}(\tau) \to \lambda K_{i_\mathrm{A}j_\mathrm{A}}(\tau).$$

In addition, it is also easily understandable why the factor λ is not multiplied to the diagonal element in the transition

matrix; from the probabilistic discussions in Eq. (A· 16), it is revealed that the diagonal elements correspond to the case without any transitions, and hence there is no count for the target transitions.

Although the basic concept of the above construction is actually the same as the generating function approach in Sect. A.1, the probabilistic interpretation of the time-evolution equation, i.e., Eq. (A· 16), would be more understandable. In addition, such probabilistic interpretation enables us to treat multiple target transition cases or more complicated cases. Indeed, the example explained in Sect. 2, the state change 'filled' → 'empty' occurs with two transition rates, i.e., $k_{\mathrm{L}}(t)$ and $k_{\mathrm{R}}(t)$. However, in Sect. 4, only one of the transitions is set to the target transition. In order to understand it, we split the element of the transition matrix into some parts. For example, we divide $K_{ij}(\tau)$ as

$$K_{ij}(\tau) = K_{ij}^{(1)}(\tau) + K_{ij}^{(2)}(\tau),$$

and then it is possible to consider that only $K_{ij}^{(2)}(\tau)$ is related to the target transition. Hence, from the probabilistic interpretation in Eq. (A· 16) we immediately obtain the following replacement

$$K_{ij}^{(1)}(\tau) + K_{i_{\mathrm{A}}j_{\mathrm{A}}}^{(2)}(\tau) \to K_{ij}^{(1)}(\tau) + \lambda K_{i_{\mathrm{A}}j_{\mathrm{A}}}^{(2)}(\tau).$$

Furthermore, multiple target transition cases can be treated in a similar manner; the usage of the inverse λ in Sect. 4.2 is also understandable in this interpretation.

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