Nonequilibrium Field Theories and Stochastic Dynamics

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1 Master Equation

Although the Gillespie algorithm can generate a single random trajectory, to understand the statistical properties of the entire stochastic process, we need a more macroscopic descriptive tool. That is the Master equation. Master equation can describe how the probability of the each state in the system evolves over time. It is a deterministic differential equation.

The history of the master equation can be traced back to the early 20th century, when physicists such as Max Born and Werner Heisenberg first introduced it in the context of quantum mechanics and statistical physics. Its core idea is to transform microscopic random processes into a macroscopic description of probability evolution, thereby enabling a systematic analysis of the overall behavior of stochastic systems.

The fundamental principle of the master equation approach is probability conservation: the rate of change of the probability that a system is in a specific state at a given time is equal to the probability flow into that state minus the probability flow out of it. This "gain–loss" balance is not only applicable to physical systems but is also widely used in many fields such as chemical reactions, population dynamics in biology, and financial modeling. The Gillespie algorithm focuses on the stochastic evolution of a single trajectory, while the master equation concerns the deterministic evolution of the entire probability distribution. The two approaches complement each other and together form an essential toolkit for the analysis of stochastic processes.

1.1 From the microscopic process to macroscopic evolution

Let us return to the microscopic description of the Poisson process. We consider the probability $p(n, t + dt)$ of the system is on the state n when $t + dt$ when we derive the Gillespie algorithm. To reach this state, there are only two possible preceding paths:

- At time t, the system is already in state $n - 1$, and then within the next dt a jump occurs. The probability of this jump is vdt. Therefore, the contribution of this path is $p(n - 1, t) \cdot vdt$.
- At time t, the system is already in state n, and then within the next dt a jump dose not occur. The probability of no jump is $1 - vdt$. Therefore, the contribution of this path is $p(n, t) \cdot (1 - vdt)$.

By adding the probabilities of these two mutually exclusive cases, we obtain the expression for $P(n, t + dt)$:

$$p(n, t + dt) = p(n - 1, t) \cdot vdt + p(n, t) \cdot (1 - vdt) \tag{1}$$

Next, we rearrange this equation.

$$\frac{p(n, t + dt) - p(n, t)}{dt} = v \cdot p(n - 1, t) - v \cdot p(n, t) \tag{2}$$

1.2 Gain–Loss Interpretation

The structure of the master equation has a very clear physical meaning: it can be viewed as a balance equation for the probability flow at each state n.

$$\frac{d}{dt}p(n, t) = v \cdot p(n - 1, t) - v \cdot p(n, t) \tag{3}$$

- **Gain term:** $v \cdot p(n-1,t)$ represents the probability flux from state $n-1$ to state n. Its magnitude is equal to the probability of the source state $p(n-1,t)$ multiplied by the transition rate v.
- **Loss term:** $v \cdot p(n,t)$ represents the probability flux from state n to state $n+1$. Its magnitude is equal to the probability of the source state $p(n,t)$ multiplied by the transition rate v.

This "gain–loss" structure is a common feature of all master equations. It is essentially a continuity equation in a discrete state space, describing that the rate of change of the probability "density" equals the net difference between the probability "fluxes" flowing into and out of the state. This also ensures the conservation of total probability.

1.3 From Stochastic Trajectories to Deterministic Evolution

Here we observe a profound conceptual shift. The Gillespie algorithm simulates a single stochastic, unpredictable trajectory $n(t)$. In contrast, the master equation is a deterministic system of differential equations, whose solution $P(n,t)$ is a smooth, predictable function.

The connection between the two lies in the fact that the master equation describes the statistical behavior of an ensemble composed of infinitely many Gillespie trajectories. If we run countless Gillespie simulations and then, at a fixed time t, compile a histogram of the values of n from all simulations, the shape of this histogram will converge to the solution $P(n,t)$ of the master equation. Therefore, the master equation bridges the microscopic randomness with the deterministic evolution of macroscopic probabilities.

Later in the lecture, we also presented the matrix form of the master equation:

$$\frac{d}{dt}\vec{p}(t) = \mathbf{W}\vec{p}(t) \tag{4}$$

Here, $\vec{p}(t)$ is a column vector whose elements are $[p(0,t), p(1,t), p(2,t), \cdots, p(n,t)]$, and $\mathbf{W}$ is a transition rate matrix. This form reveals that the master equation is essentially a system of linear ordinary differential equations, paving the way for using linear algebra tools, such as eigenvalue decomposition, to solve the system dynamics.

2 Solving the Master equation by generating function

Although the master equation has an elegant form, it is essentially an infinite-dimensional system of coupled ordinary differential equations, and solving it directly is usually very difficult. To address this challenge, a powerful tool has been developed in mathematical physics — the generating function.

2.1 Definition and Transformation of the Generating Function

The core idea of the generating function is to perform a nonlinear summation of an infinite sequence of probabilities and encode them into a single function $G(s,t)$:

$$G(s,t) = \sum_{n=0}^{\infty} p(n,t)s^n \tag{5}$$

Here the variable s is an auxiliary variable without direct physical meaning, but it acts like a "ledger": the coefficient of s^n in $G(s,t)$ is exactly the probability $p(n,t)$ which we are interested in. The magical power of the generating function lies in its ability to transform the difference operations in the master equation (such as $p(n,t)$) into algebraic operations. We multiply both sides of the master equation by s^n, and then sum over all n:

$$\sum_{n=0}^{\infty} \frac{d}{dt}p(n,t)s^n = \sum_{n=0}^{\infty} v \cdot p(n-1,t)s^n - \sum_{n=0}^{\infty} v \cdot p(n,t)s^n \tag{6}$$

Let us handle this equation term by term:

- **Left side:** Since summation and differentiation can be interchanged, we obtain

$$\sum_{n=0}^{\infty} \frac{d}{dt} p(n,t) s^n = \frac{d}{dt} \sum_{n=0}^{\infty} p(n,t) s^n = \frac{d}{dt} G(s,t) \tag{7}$$

- **The second term in the right side:**

$$\sum_{n=0}^{\infty} v \cdot p(n,t) s^n = v \cdot \sum_{n=0}^{\infty} p(n,t) s^n = v \cdot G(s,t) \tag{8}$$

- **The first term in the right side:** This is the most crucial step. We make a change of variables, letting $m = n - 1$, thus $n = m + 1$

$$\sum_{n=0}^{\infty} v \cdot p(n-1,t) s^n = \sum_{m=0}^{\infty} v \cdot p(m,t) s^{m+1} = v \cdot s \cdot \sum_{m=0}^{\infty} p(m,t) s^m = v \cdot s \cdot G(s,t) \tag{9}$$

By combining these three terms, we have successfully transformed the infinite-dimensional system of ordinary differential equations into a single-variable partial differential equation:

$$\frac{d}{dt} G(s,t) = v \cdot s \cdot G(s,t) - v \cdot G(s,t) \tag{10}$$

2.2 Solving and Result Restoration/Reconstruction

The equation for $G(s,t)$ is a simple first-order linear ordinary differential equation (for fixed s), which we can solve directly by integration. First, we need an initial condition. Typically, we assume the system starts from state n at $t = 0$, i.e., $p(n,0) = \delta_{n,0}$. This initial condition corresponds in the generating function space to:

$$G(s,0) = \sum_{n=0}^{\infty} p(n,0) s^n = p(0,0) s^0 = 1 \tag{11}$$

Now, by solving the differential equation $\frac{dG}{G} = v(s-1)dt$ and integrating from $t = 0$ to t, we obtain:

$$\ln(G(s,t)) - \ln(G(s,0)) = v(s-1)t \rightarrow G(s,t) = \exp(v(s-1)t) \tag{12}$$

We have thus obtained the analytical expression for the generating function. The final step is how to "decode" the probability $p(n,t)$ from $G(s,t)$. According to the definition of the Taylor expansion, $p(n,t)$ is precisely the coefficient of s^n in the Taylor expansion of $G(s,t)$ at $(s = 0)$, divided by $n!$. A more intuitive approach is to directly expand $G(s,t)$:

$$G(s,t) = \sum_{n=0}^{\infty} \frac{(vt)^n}{n!} s^n e^{-vt} = \sum_{n=0}^{\infty} [e^{-vt} \frac{(vt)^n}{n!}] s^n. \tag{13}$$

By comparing this expansion term by term with the generating function definition $G(s,t) = \sum_{n=0}^{\infty} p(n,t) s^n$, we immediately obtain the solution of the master equation:

$$p(n,t) = e^{-vt} \frac{(vt)^n}{n!} \tag{14}$$

This is exactly the familiar Poisson distribution with mean $(\lambda = vt)$.

2.3 The Power of Generating Functions: Calculating Moments

Generating functions not only allow us to solve the master equation analytically, but they also provide a straightforward way to compute the moments of the distribution. Recall the definition:

$$G(s,t) = \sum_{n=0}^{\infty} p(n,t)s^n. \tag{15}$$

The moments of the random variable $n(t)$ can be obtained by differentiating the generating function with respect to s and then evaluating at $s = 1$:

- **Mean (first moment):**

$$\langle n(t)\rangle = \sum_{n=0}^{\infty} np(n,t) = \left.\frac{\partial G(s,t)}{\partial s}\right|_{s=1} = vt\exp\left(vt(s-1)\right)|_{s=1} = vt \tag{16}$$

- **Second moment:**

$$\langle n^2(t)\rangle = \left.\frac{\partial^2 G(s,t)}{\partial s^2}\right|_{s=1} + \langle n(t)\rangle \tag{17}$$

- **Variance:**

$$\mathrm{Var}[n(t)] = \langle n^2(t)\rangle - \langle n(t)\rangle^2 \tag{18}$$

For the Poisson generating function $G(s,t) = e^{vt(s-1)}$, we immediately get:

$$\langle n(t)\rangle = vt, \quad \mathrm{Var}[n(t)] = vt. \tag{19}$$

2.4 Summary

This lecture guided us to a deeper understanding of stochastic processes from three complementary perspectives: the Gillespie algorithm, the master equation, and the generating function. Together, they form a powerful and complete theoretical and computational framework.

- **Gillespie Algorithm**: Provides a numerical simulation perspective. It is an event-driven and exact algorithm that generates individual trajectories of stochastic processes, allowing us to directly observe how randomness manifests.
- **Master Equation**: Provides a probability evolution perspective. It is a deterministic differential equation that describes how the probabilities of the system being in different states evolve over time, capturing the statistical laws of the entire ensemble of stochastic trajectories.
- **Generating Function**: Provides an analytical solution perspective. It is a powerful mathematical tool that transforms the complex master equation (an infinite-dimensional system of differential equations) into a simple single equation, enabling the derivation of analytic probability distributions and the convenient calculation of statistical moments.

Each of these three approaches has its own focus, and together they provide a solid foundation for analyzing a wide range of stochastic phenomena—from particle motion in physics to population dynamics in biology.

3 Linear Death Process: The Basis of Stochastic Population Models

3.1 Application: An Introduction to Population Dynamics

Consider the simplest model: the Simple Death Process. This process can be expressed in a chemical reaction–like form:

$$A \to 0 \tag{20}$$

This indicates that individuals of species A die or disappear from the system at a certain rate. The key point here is the physical meaning of λ : it is the per capita death rate.

This means that if there are currently n individuals in the system, then the total death rate of the population is $n\lambda$. This is a crucial distinction: the transition rate is no longer a constant but depends on the current state n of the system. Such **state-dependent rates** are a common and important concept in stochastic modeling.

We can once again use the "Gain–Loss" logic to construct the master equation for this process. What we are interested in is the probability $p(n,t)$ that the population size is n at time t.

- Gain term (GAIN): For the system to reach state n at time t, it must have come from state $n+1$ through a single death event. When the population size is $n+1$, the total death rate is $(n+1)\lambda$. Therefore, the probability flux from state $n+1$ into state n is $(n+1)\lambda p(n+1,t)$
- Loss term (LOSS): If the system is currently in state n. it will leave this state due to a death event. In this case, the total death rate is $n\lambda$. Therefore, the probability flux out of state n is $n\lambda p(n,t)$

Combining the gain and loss terms, we obtain the master equation for the simple death process:

$$\frac{d}{dt}p(n,t) = (n+1)\lambda p(n+1,t) - n\lambda p(n,t). \tag{21}$$

The structure of this equation is similar to the master equation for the Poisson process, but the transition rate has changed from a constant λ to the state-dependent form $n\lambda$. This seemingly simple modification leads to a qualitative change in the system's dynamical behavior. This is an infinite-dimensional coupled system of ordinary differential equations (for $(n = 0, 1, 2, \dots)$), making its direct solution quite challenging.

3.2 Exact solution: reveals the binomial nature of survival

Instead of directly solving the master equation, let us start with a simpler problem and then gradually generalize.

The survival of the single body First, consider the case where there is only one individual initially $n_0 = 1$. What is the probability that this individual is still alive at time t? This is a classic exponential waiting-time problem. In any infinitesimal time interval dt, the probability of its death is λdt. Therefore, the probability $p(t)$ that it is still alive at time t satisfies:

$$\frac{d}{dt}p(t) = -\lambda p(t) \tag{22}$$

The solution is $p(t) = \exp(-\lambda t)$. Accordingly, the probability that it has died by time t is $q(t) = 1 - p(t) = 1 - \exp(-\lambda t)$,

Generalization to N_0 individuals Now, let us return to the case with an initial population of N_0. A core assumption of the linear death process is that the death events of each individual are independent. The death of one individual does not affect the probability of death of another. This implies that, at time t, the survival of the entire population can be viewed as N_0 independent "Bernoulli trials."

Each trial corresponds to an initial individual, and the outcome of each trial has only two possibilities:

- The individual survives until time t, with probability $p(t) = \exp(-\lambda t)$
- The individual dies until time t, with probability $q(t) = 1 - \exp(-\lambda t)$

We are interested in the probability that, out of N_0 trials, exactly N are "successes" (i.e., N individuals survive). This is precisely the definition of the binomial distribution! Therefore, we can directly write its probability distribution:

$$p(n,t) = \binom{N_0}{n}[p(t)]^N[q(t)]^{N_0-N} = \binom{N_0}{n}(e^{-\lambda t})^n(1-e^{-\lambda t})^{N_0-N}. \tag{23}$$

Once we know that the probability distribution is binomial, we can use its well-known properties to compute the mean and variance. For a binomial distribution with parameters N_0 and $p(t) = \exp(-\lambda t)$, the mean is

$$\langle n \rangle = N_0 p(t) = N_0 e^{-\lambda t}, \tag{24}$$

and the variance is

$$\mathrm{Var}(n) = N_0 p(t)(1 - p(t)) = N_0 e^{-\lambda t}(1 - e^{-\lambda t}). \tag{25}$$

Here we uncover a crucial conclusion: the mean of the stochastic process $\langle n \rangle$, exactly coincides with the deterministic mean-field solution we derived earlier! This is a beautifully general result for all linear processes. It tells us that the deterministic equation indeed captures the system's average behavior correctly.

However, the variance $\mathrm{Var}(n)$ is an entirely new quantity, arising purely from stochasticity. It quantifies the magnitude of "population noise"—that is, the extent to which actual population trajectories fluctuate around the mean due to the randomness of individual death events. This is information that the mean-field approach cannot capture at all.

3.3 Verification by computation: simulating the linear death process

We can modify the previous Gillespie algorithm to simulate this state-dependent death process. The only essential change is that, when computing the waiting time, the rate used is no longer a constant but a function of the current population size n.

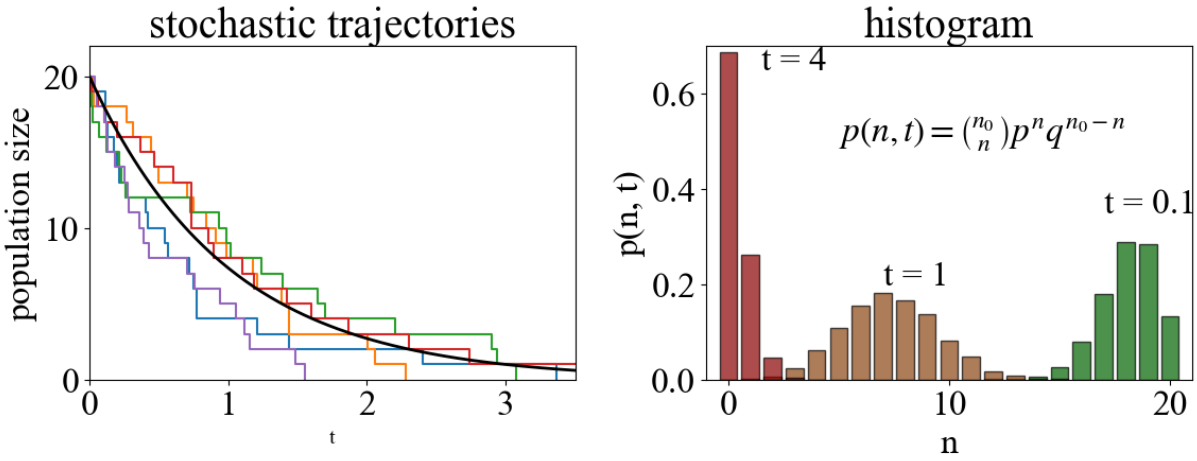

Figure 1:

Right panel (histogram): This figure shows the probability distribution of the population size at three different time points $t = 0.1, 1, 4$. The bars represent the empirical distributions obtained from tens of thousands of Gillespie simulations. As time progresses, the peak of the distribution shifts to the left (indicating a decrease in the average population) and the distribution widens (reflecting increased relative uncertainty). Eventually, at long times, most simulations end with population extinction $n = 0$. This dynamic behavior perfectly matches the binomial distribution we derived.

Left panel (stochastic trajectories): This figure shows three independent simulation trajectories (colored step lines). Each trajectory represents a possible history. The smooth black curve corresponds to the deterministic solution $n(t) = n_0 \exp(-\lambda t)$, i.e., the mean of the stochastic process. This figure intuitively illustrates the key feature of stochastic processes: individual realizations (trajectories) are random and discrete, but the average over many realizations converges to the deterministic mean-field solution.

4 Lotka–Volterra Process: Simulating Predator–Prey Interactions

References