From Events to Equations

Modeling Out-of-Equilibrium Systems

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Table of contents

1 Formalizing Discrete-Event Stochastic Systems **1**
1.1 State Space: What the System Is . . . 1
1.2 Event Set: What Can Happen . . . 2
1.3 Transition Rates: How Likely and When . . . 2
1.4 Time and the Poisson Clock . . . 2
1.5 Evolution as a Stochastic Process . . . 3
1.6 Realizations and Ensemble Behavior . . . 3

2 Stochastic Master Equation: Evolution of the Probability Distribution **4**
2.1 Gain–Loss Structure . . . 4
2.2 Why This Matters . . . 5

3 Example 1: Pure Birth Process **5**
3.1 Model Setup . . . 5

4 Expected Observables and Mean-Field Approximation **6**
4.1 Defining an Observable . . . 6
4.2 Exact Result (Moment Evolution) . . . 7
4.3 Heuristic + Step-by-Step Breakdown . . . 8
4.4 Mean-Field Approximation . . . 9
4.5 Derivation from the Stochastic Master Equation . . . 10

5 Example 2: Pure Birth Process revisted **11**

6 Aggregation Dynamics **11**

1 Formalizing Discrete-Event Stochastic Systems

A systems-level view: what defines the system, what can happen, and how often.

1.1 State Space: What the System Is

We define the state space Σ as the set of all possible configurations the system can be in.

This could be:

- a vector of counts (e.g., $\mathbb{N}^d$ in chemical systems),
- a network structure,
- a set of labeled groups,
- or any structured object that encodes the relevant degrees of freedom.

At any time t, the system is in some state $S(t) \in \Sigma$ — this is the complete description of the system at that moment.

1.2 Event Set: What Can Happen

We define a set of discrete events $\mathcal{E} = \{R_k\}$.

Each event R_k is a transformation:

$$R_k : \Sigma \to \Sigma$$

That is, it modifies the current state into a new one.

These can represent things like:

- merging clusters,
- adding or removing links,
- opinion changes,
- or particle interactions.

Together, the event set describes what transitions are possible in your model.

1.3 Transition Rates: How Likely and When

We assign a rate $\omega_k(S)$ to each event R_k, which tells us how likely that event is to occur per unit time, when the system is in state S.

Formally:

$$\omega_k : \Sigma \to \mathbb{R}_{\geq 0}$$

Rates are where we encode the model's assumptions and mechanisms.
They can depend on local structure, global statistics, or features of the state.

1.4 Time and the Poisson Clock

Each event is assumed to occur according to a Poisson process with rate $\omega_k(S)$.

That is: - Each event has its own "clock" that ticks randomly. - The time until the next tick is drawn from an exponential distribution:

$$\tau_k \sim \text{Exp}(\omega_k(S))$$

We imagine all event clocks running in parallel — the one that "rings" first determines: - **Which event occurs** - **When it happens**

This implies:

- Events are independent
- The system has no memory
- The statistics are stationary in time

These assumptions define a very general and powerful class of models.

1.5 Evolution as a Stochastic Process

Having defined $(\Sigma, \mathcal{E}, \omega)$, we've specified:

- what the system is,
- what can happen,
- how likely and when it will happen.

This gives us a **continuous-time, discrete-event stochastic process**, also known as a **Markov jump process**.

1.6 Realizations and Ensemble Behavior

A stochastic process is a random evolution of the system over time:

$$\{S(t)\}_{t \geq 0}$$

Each **trajectory** (or **realization**) is one possible outcome:

$$(S_0, t_0) \to (S_1, t_1) \to (S_2, t_2) \to ...$$

It tells us **what happened**, and **when** — based on random choices made by the system.

But to understand the full dynamics, we don't just want one realization.
We need to consider **many trajectories** and track how the **distribution over states** evolves in time.

2 Stochastic Master Equation: Evolution of the Probability Distribution

One approach to study the dynamics of the system is through the **Stochastic Master Equation** (SME).
It gives a complete description of the system's evolution in time — telling us, for each state S, how the probability $P(S,t)$ increases or decreases due to possible events.

We define the transition rate from one state to another as:

$$W_{S_1 \to S_2} = \sum_{k\,:\,R_k(S_1)=S_2} \omega_k(S_1)$$

This means:
- for a given pair of states S_1 and S_2,
- we sum over all events R_k that, when applied to S_1, produce S_2,
- and we weight each by its rate $\omega_k(S_1)$.

2.1 Gain–Loss Structure

We now describe how $P(S,t)$ changes over time:

Gain term:

Probability flowing **into** state S from other states $S' \in \Sigma$ due to events that lead to S:

$$\text{Gain} = \sum_{S' \in \Sigma} W_{S' \to S}\, P(S',t)$$

Loss term:

Probability flowing **out of** state S into other states $S' \in \Sigma$ due to events that start in S:

$$\text{Loss} = \sum_{S' \in \Sigma} W_{S \to S'}\, P(S,t)$$

Putting it together, the **Stochastic Master Equation** is:

> **Stochastic Master Equation**
>
> $$\frac{dP(S,t)}{dt} = \sum_{S' \in \Sigma} \left[W_{S' \to S}\, P(S',t) - W_{S \to S'}\, P(S,t) \right]$$

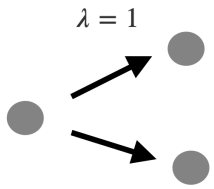
This equation describes the **net rate of change** in the probability of being in state S.

2.2 Why This Matters

- The SME tracks the **probability flow** in and out of each state.
- It is **exact** — it fully characterizes the stochastic dynamics of the system.
- In practice, the equation is often **too large to solve directly**.
- But it forms the foundation for:
  - **Stochastic simulation algorithms** (like Gillespie's),
  - **Approximations** (mean-field, moment closures),
  - And deeper theoretical insights (steady states, fluctuations, etc.)

3 Example 1: Pure Birth Process

Let's apply the Stochastic Master Equation to a simple system: a **pure birth process**.



3.1 Model Setup

States, Events, and Rates

- **State space**: The system is in state n when there are n particles.

$$S = \{n \in \mathbb{N}\}$$

- **Event**: a new particle is added (birth event)

$$R(n) = n + 1$$

- **Rate function**: each of the n particles produces a new one independently at rate $\lambda = 1$

$$\omega(n) = n\lambda = n$$

Let $P_n(t)$ denote the probability that there are n particles at time t.

Stochastic Master Equation

Using the SME, we can write the time evolution of $P_n(t)$ as:

$$\frac{dP_n(t)}{dt} = \underbrace{(n-1)\,P_{n-1}(t)}_{\text{Gain from } n-1\to n} - \underbrace{n\,P_n(t)}_{\text{Loss from } n\to n+1}$$

- **Gain**: the system transitions from state $(n-1)$ to n
- **Loss**: the system leaves state n due to a birth

This equation describes how probability flows **into and out of** each state over time.

4 Expected Observables and Mean-Field Approximation

The Stochastic Master Equation (SME) gives a complete description of system dynamics: it tracks the full probability distribution over the state space.

But this is often intractable for large or structured systems.

In many cases, we are more interested in the *expected behavior*, especially when fluctuations are small or we want coarse-grained insight. This leads to a deterministic ODE or a mean-field approximation, where we model the behavior using ordinary differential equations instead of full distributions.

4.1 Defining an Observable

We define a real-valued observable (or measure) as:

$$f : \Sigma \to \mathbb{R}$$

It maps each state S to some quantity of interest. For example, $f(S)$ might be: - the number of infected individuals, - the size of a particular cluster, - or the number of links in a network.

In many systems, we track **multiple observables simultaneously**. In that case:

$$f : \Sigma \to \mathbb{R}^n$$

This is common in models with multiple interacting components — for example, **chemical species counts** or **multi-type populations**, where each component's count evolves in time and may be

coupled to others.

The expected value of this observable at time t is:

$$\bar{f}(t) = \langle f(S) \rangle(t) = \sum_{S \in \Sigma} f(S) \cdot P(S, t)$$

Our goal is to understand how this expected value evolves over time:

$$\frac{d}{dt}\bar{f}(t) = \sum_{S \in \Sigma} f(S) \cdot \frac{d}{dt} P(S, t)$$

4.2 Exact Result (Moment Evolution)

We now derive how the expected value of an observable evolves over time using our event-based formalism.

Recall that for a real-valued observable $f : \Sigma \to \mathbb{R}$, the expected value at time t is:

$$\bar{f}(t) = \langle f(S) \rangle(t) = \sum_{S \in \Sigma} f(S) \cdot P(S, t)$$

Taking the time derivative gives:

$$\frac{d}{dt}\bar{f}(t) = \sum_{S \in \Sigma} f(S) \cdot \frac{d}{dt} P(S, t)$$

We now express the right-hand side using our model of the system's dynamics in terms of events.

Each event R_k changes the system from state S to $R_k(S)$ with rate $\omega_k(S)$. The corresponding change in the observable is:

$$\Delta_k f(S) = f(R_k(S)) - f(S)$$

This leads to the exact time evolution equation for the expected value:

$$\frac{d}{dt}\bar{f}(t) = \sum_k \langle \Delta_k f(S) \cdot \omega_k(S) \rangle$$

This expression says that the rate of change of the expectation is the sum over all events k of the expected contribution of each event to the observable's change, weighted by how likely that event is to occur in state S. This equation is still exact and follows directly from the master equation formalism — we've just shifted from tracking $P(S, t)$ to tracking $\bar{f}(t)$.

Note that the bracket notation $\langle \cdot \rangle$ denotes an average over the entire state space Σ with respect to the probability distribution $P(S,t)$. As a result, any quantity inside the brackets is no longer dependent on the specific state S, but instead reflects a system-wide expected value at time t.

4.3 Heuristic + Step-by-Step Breakdown

What happens when an event R_k occurs?

- Change in State:

$$S \to R_k(S)$$

- Change in Measure:

$$f(S) \to f(R_k(S))$$

- Net change:

$$\Delta_k f(S) = f(R_k(S)) - f(S)$$

Expected change from one event:

- The process R_k has a rate $\omega_k(S)$, giving the probability per unit time that it occurs.
- In a small time dt, the expected contribution of R_k is:

$$\Delta_k f(S) \cdot \omega_k(S) \cdot dt$$

This is still conditional on being in state S.

Average over all states and processes:

To find the overall expected change, we average over all states, then all events:

$$\frac{d}{dt}\langle f(S) \rangle(t) = \sum_k \sum_S \Delta_k f(S) \cdot \omega_k(S) \cdot P(S,t) = \sum_k \langle \Delta_k f(S) \cdot \omega_k(S) \rangle$$

This gives us the **exact** time evolution of the first moment (mean) of $f(S)$.

What we have here:

1. Compute change in observables due to each event.

2. Multiply it by how often that event occurs at each state.

3. Average over all states.

4. Sum up over all processes.

4.4 Mean-Field Approximation

In many systems, solving the exact dynamics is intractable due to the size or complexity of the state space. Tracking the full distribution $P(S,t)$ may be computationally or analytically prohibitive.

Instead, we often ask:

> Can we approximate how the system evolves on average, by assuming it behaves like its **typical** or **average** state?

This leads to the **mean-field approximation**, where we replace state-dependent quantities with their values at the average state $\bar{S}$.

Specifically, we approximate:

$$\langle \Delta_k f(S) \cdot \omega_k(S) \rangle \approx \Delta_k f(\bar{S}) \cdot \omega_k(\bar{S})$$

So the equation for the evolution of the expected observable becomes:

$$\frac{d}{dt}\bar{f}(t) \approx \sum_k \Delta_k f(\bar{S}) \cdot \omega_k(\bar{S})$$

This approximation **ignores fluctuations and correlations** — it treats the system as if it always evolves deterministically through its average state. It's often valid when: - The system is large (law of large numbers), - Fluctuations are small or short-lived, - Correlations between components are weak.

Mean-field models are powerful because they reduce high-dimensional stochastic systems to lower-dimensional deterministic equations. While they miss some variability, they often capture the **dominant trends** and provide useful analytical insight into system behavior.

4.5 Derivation from the Stochastic Master Equation

We can arrive at the same result we obtained from the heuristic argument — the time evolution of the expected value of an observable — directly and rigorously from the Stochastic Master Equation (SME).

Start with the expected value of an observable f:

$$\frac{d}{dt}\bar{f}(t) = \sum_{S} f(S) \cdot \frac{d}{dt} P(S,t)$$

Recall from the SME:

$$\frac{dP(S,t)}{dt} = \sum_{S' \in \Sigma} \left[W_{S' \to S} \cdot P(S',t) - W_{S \to S'} \cdot P(S,t) \right]$$

where the transition rate between two states is defined as:

$$W_{S_1 \to S_2} := \sum_{k : R_k(S_1) = S_2} \omega_k(S_1)$$

Plugging into the time derivative:

$$\frac{d}{dt}\bar{f}(t) = \underbrace{\sum_{S} \sum_{S'} f(S) \cdot W_{S' \to S} \cdot P(S',t)}_{\text{gain}} - \underbrace{\sum_{S} \sum_{S'} f(S) \cdot W_{S \to S'} \cdot P(S,t)}_{\text{loss}}$$

> **Take Note**
>
> $$\sum_{S_2} \sum_{k:\, R_k(S_1) = S_2} \equiv \sum_{k}$$
>
> Since the inner sum only includes indices that result in a given state, and the outer sum goes over all possible resulting states, the total sum ends up covering all indices — just grouped differently.

Gain Term

$$= \sum_S \sum_{S'} f(s) \Big(\sum_{k:R_k(S')=S} w_k(S') \Big) P(S',t) \tag{1}$$

$$= \sum_{S'} f(R_k(S')) \underbrace{\sum_S \sum_{k:R_k(S')=S}}_{\sum_k} \omega_{S'} P(S',t) \tag{2}$$

$$= \sum_{S'} \sum_k f(R_k(S'))\omega_k(S')P(S',t) \tag{3}$$

$$= \sum_S \sum_k f(R_k(S))\omega_k(S)P(S,t) \tag{4}$$

Loss Term

$$= \sum_S f(S) \Big(\underbrace{\sum_{S'} \sum_{k:R_k(S)=S'}}_{\sum_k} w_k(S) \Big) P(S,t) \tag{5}$$

$$= \sum_{S'} \sum_k f(S)\omega_k(S)P(S,t) \tag{6}$$

Putting It Together

$$\frac{d}{dt}\bar{f}(t) = \sum_k \sum_S (f(R_k(S)) - f(S))\omega_k(S)P(S,t) \tag{7}$$

$$= \sum_k \langle \Delta_k f(S)\omega_k(S) \rangle \tag{8}$$

5 Example 2: Pure Birth Process revisted

6 Aggregation Dynamics