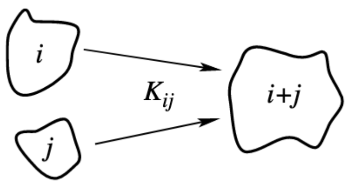
From Events to Equations

Modeling Out-of-Equilibrium Systems

Sara Maria El Oud

Building Blocks of Stochastic Dynamics: State, Events, and Evolution

Irreversible Aggregation



$$K_{ij} \equiv \text{rate at which a cluster of size } i \text{ merges with a cluster of size } j$$

$$n_k \equiv \text{number of clusters of size } k$$

Cluster Size Distribution: $\vec{n} = (n_1, n_2, n_3, \ldots, n_N) = \{n_i \mid i \in [1, N]\}$

- **Total Size of System** : $\sum_k k \times n_k = N$
- **Total Number of Clusters**: $\sum_k n_k = N_c$

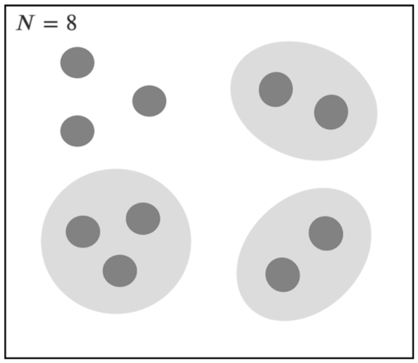
States, Events, and Transition Rates

State Space (Σ)

$$\Sigma = \left\{ \vec{n} \in \mathbb{Z}^N_{\geq 0} \,\middle|\, \sum_k k n_k = N \right\}$$

State ($S \in \Sigma$) $\quad S = \vec{n}$

$$\begin{aligned} \vec{n} &= [n_1, n_2, n_3, n_4, n_5, n_6, n_7, n_8] \\ &= [3, 2, 1, 0, 0, 0, 0, 0] \end{aligned}$$

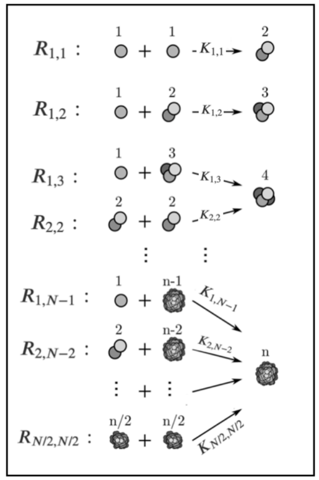


Event Space ($\mathcal{E}$)

$$\mathcal{E} = \{ R_{i,j} \mid i, j \in [1, N] \}$$

Event ($R_k : \Sigma \to \Sigma$)

$$R_{ij}(n_k) : \begin{cases} n_i \to n_i - 1 \\ n_j \to n_j - 1 \\ n_{i+j} \to n_{i+j} + 1 \end{cases}$$



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

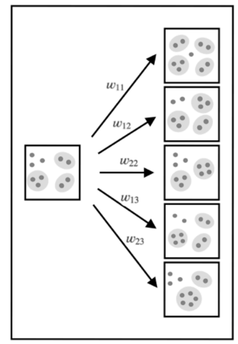
$$\omega_{ij} = \begin{cases} \frac{1}{2} n_i (n_i - 1) K_{ij} & i = j \\ n_i n_j K_{ij} & i \neq j \end{cases}$$

Competing Poisson Processes

(more on this in Gillespie Algorithm)

$$P(\text{event between } i \text{ and } j) = \frac{w_{ij}}{\Omega}$$

$$(S_1, t_1) \to (S_2, t_2)$$



Total Rate

$$\Omega = \sum_{\forall k} w_k$$

Independent Poisson Process

$$\tau_k \sim exp(\omega_k)$$

Waiting Time Distribution

$$P(\tau) = \Omega(\tau) exp(-\Omega \tau)$$

Evolution as a Stochastic Process

- State Space: $\Sigma \rightarrow$ what the system is
- Event Space: $\mathcal{E} \rightarrow$ what can happen
- Transition Rates: $\omega \rightarrow$ how likely and when it happens

continuous-time, discrete-event stochastic process

$\equiv$

Markov Jump Process

Stochastic Process

Time Evolution of System State

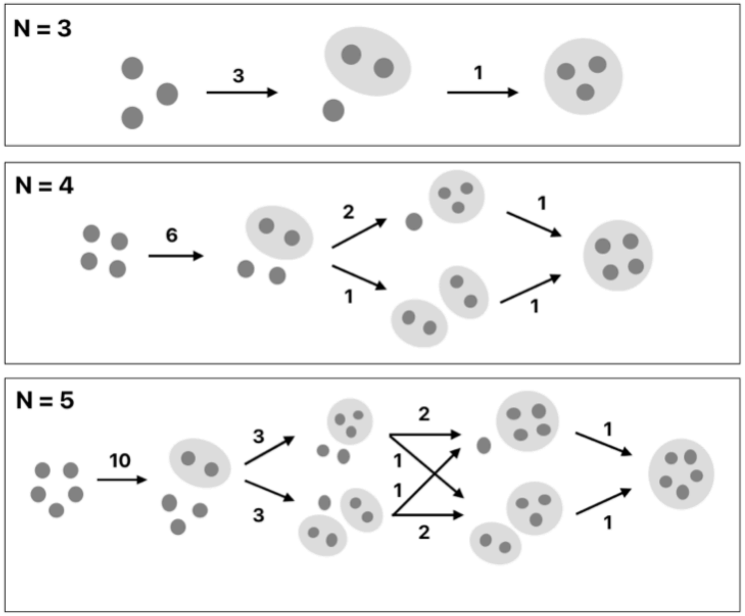
$\{S(t)\}$ for $t \geq 0$

Trajectory/Realization

One Possible Path

$(S_0, t_0) \rightarrow (S_1, t_1) \rightarrow (S_2, t_2) \rightarrow \ldots$

Example Trajectories with Rates



Stochastic Master Equation

Evolution of the Probability Distribution

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

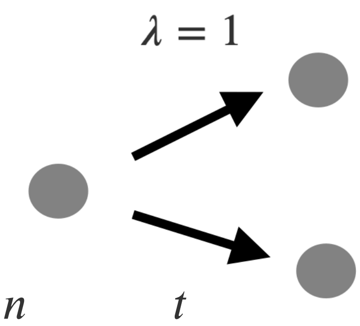
$$W_{S_1 \to S_2} = \sum_{k\,:\,R_k(S_1)=S_2} \omega_k(S_1)$$

One way to describe the dynamics is through the **Stochastic Master Equation**, which tells us how the probability $P(S, t)$ changes over time due to possible events.

$$\frac{dP(S,t)}{dt} = \underbrace{\sum_{S' \in \Sigma} W_{S' \to S}\, P(S', t)}_{\text{Gain}} - \underbrace{\sum_{S' \in \Sigma} W_{S \to S'}\, P(S, t)}_{\text{Loss}}$$

Birth Process: Setup

- We define the system as:
  - **State space**: $\Sigma = \{n \in \mathbb{N}\}$
  - **Event**: $R(n) = n + 1$
  - **Rate**: $\omega(n) = n$
- Let $P_n(t)$ be the probability that the system is in state n
- The Stochastic Master Equation becomes:



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