2. The Master Equation. Simulation with the Gillespie Algorithm.

- Stochastic process: variable(s) evolving in time in a non-deterministic manner.
- Examples: lightning formation (dielectric breakdown), brownian motion, chemical reactions, bacterial growth, species interaction in ecology, financial markets, ...
- Markov process: type of stochastic process in which the probability of each event depends only on the previous event (NO MEMORY).
  - ↳ modelled through the "Chapman-Kolmogorov eq".
- MASTER EQUATION: differential eq. for a stochastic Markov process with time as a continuous variable:

  $\vec{n}(t) \equiv$ state of the system at time t.

  $P(\vec{n}, t \mid \vec{n}_0, t_0) \equiv$ prob. of finding the system at state $\vec{n}$ at time t, having the initial conditions $\vec{n}(t=t_0) = \vec{n}_0$

Note: we will keep $\vec{x}$ for continuous variables and use $\vec{n}$ instead for discreet variables.

EXAMPLE: the susceptible-infected-susceptible model:

Well-mixed system of N individuals in states S or I; dynamics evolves stochastically according to the following processes ("reactions"):

$$I \xrightarrow{\mu} S \quad ; \qquad I + S \xrightarrow{\lambda} I + I$$

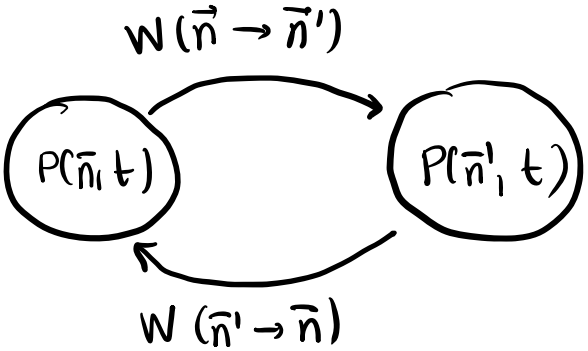
where μ, λ are the corresponding "rates" per interaction (see below).

Note: well-mixed = the dynamics is based only on the concentration of our "chemical species", not on their specific location. This is a good simplification when most interactions are "non-reactive" (e.g. elastic collisions...). Otherwise we might need to use a spatially explicit description...

- The Master eq. is a continuity equation for the change of $P(\vec{n}, t \mid \vec{n}_0, t)$ in time.
(see refs. for a more formal derivation).

Note: for convenience I will omit the initial cond.

$$\partial_t P(\vec{n}, t) = \underbrace{+ \text{ incoming flux of probability}}_{} \; \underbrace{- \text{ outgoing flux of probability}}_{}$$



with $W(\vec{n} \to \vec{n}') \cdot \Delta t$ the prob. of going from $\vec{n} \to \vec{n}'$ during a small interval Δt

$W(\vec{n} \to \vec{n}')$ = "rate" of prob].

Then, $\partial_t P(\vec{n}, t) = \sum_{\vec{n}'} [\, W(\vec{n}' \to \vec{n})\, P(\vec{n}', t) - W(\vec{n} \to \vec{n}')\, P(\vec{n}, t) \,]$.

Example (SIS): $\vec{n} = (n_I, n_S) = (n_I, N - n_I)$; then for simplicity $n_I \equiv n$.

"reaction" 1 $\quad I \xrightarrow{\mu} S$ ("unimolecular reaction")

$W(n \to n-1) \propto n$: "the more I ind. I have, the more likely the reaction".

$\hookrightarrow W(n \to n-1) = \mu n$, with $\mu \equiv$ rate per particle

"reaction" 2 $\quad I + S \longrightarrow I + I$ ("bimolec. reaction")

$W(n \to n+1) \propto n \cdot \frac{n_S}{N} = \frac{N-n}{N}$ (this takes into account the prob. that every I finds one S in the system)

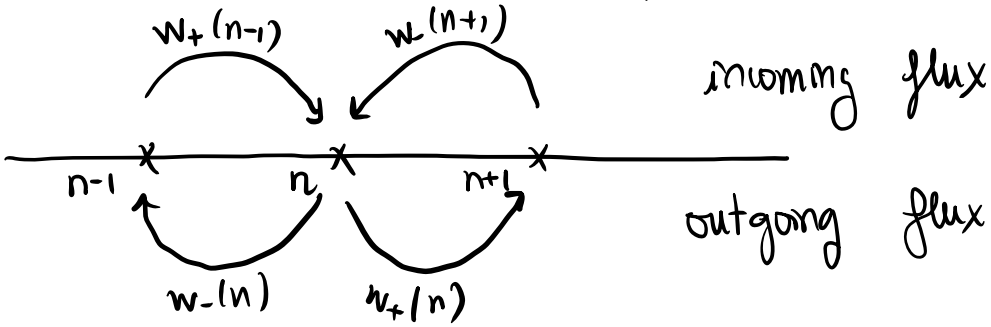
$\hookrightarrow W(n \to n+1) = \lambda n \left(1 - \frac{n}{N}\right)$

with $\lambda \equiv$ rate of prob. per pair of particles.

Note: Generally, rates W should scale linearly with the system size.

For simplicity, $W(n \to n-1) \equiv W_-(n)$ ("one-step process").
$W(n \to n+1) \equiv W_+(n)$

Then we write the Master equation:

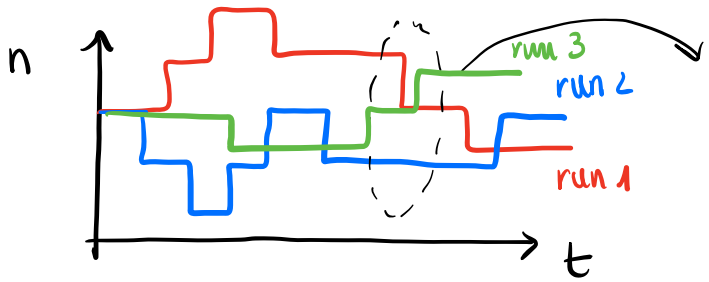


$$\partial_t P(n,t) = W_{+1}(n-1)\,P(n-1,t) + W_{-1}(n+1)\cdot P(n+1,t) - W_{+1}(n)\,P(n,t) - W_{-1}(n)\,P(n,t).$$

+ initial conditions of $P(n_0, t_0)$ (e.g. $P(n_0, t_0) = \delta_{n,n_0}$)

- This is in gral. difficult to solve analytically or even numerically.

↳ Much better to have an algorithm that gives us <u>stochastic trajectories</u> of $n(t)$ compatible with $P(n,t \mid n_0, t_0)$.



I can compute numerically $P(n,t)$ numerically

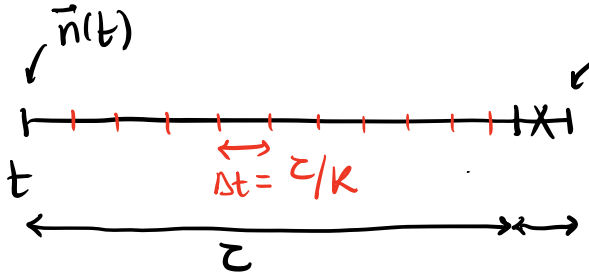
2.1. The Gillespie algorithm.

Main idea In order to track $\bar{n}(t)$, all we need to know is:

- <u>when</u> next reaction will take place.
- <u>which</u> reaction will take place (to update $\bar{n}(t)$ accordingly).

Then, $p(\bar{n}, t \mid \bar{n}_0, t_0) \longrightarrow p(\tau, j \mid \bar{n}, t)$,

with $p(\tau, j \mid \bar{n}, t)\,\Delta\tau \equiv$ prob. reaction j occurs during a small interval $[t+\tau,\ t+\tau+\Delta\tau)$



- We can compute $P(\tau, j \mid \bar{n}, t)$:

$$P(\tau, j \mid \bar{n}, t)\,\Delta\tau = \text{prob. nothing happens during } [t, t+\tau] \times \text{prob. reaction } j \text{ happens in } [t+\tau, t+\tau+\Delta\tau]$$

$$\lim_{K\to\infty} P(\tau, j \mid \bar{n}, t)\,\cancel{\Delta\tau} = \left[1 - \sum_j w_j(\bar{n})\cdot\Delta t\right)^K \cdot\ w_j(\bar{n})\,\cancel{\Delta\tau}$$

Por qué elevar a k?

$$\lim_{K\to\infty} P(\tau, j \mid \bar{n}, t) = \left(1 - \sum_j w_j(\bar{n}) \frac{\tau}{K}\right)^K w_j(\bar{n})$$

$$= \exp\left(-\sum_j w_j(\bar{n}) \cdot \tau\right) \cdot w_j(\bar{n}) .$$

- If we look at $P(\tau \mid \bar{n}, t) \equiv \sum_j P(\tau, j \mid \bar{n}, t) =$ prob. distrib. ANY reaction j takes place at interval $[t+\tau,\ t+\tau+d\tau]$

$$P(\tau \mid \bar{n}, t) = \sum_j w_j(\bar{n}) \cdot e^{-\sum_j w_j \cdot \tau}$$

↳ $\tau \sim$ exp. distribution of mean $w_0(\bar{n}) \equiv \sum_j w_j(\bar{n})$

- $$\frac{p(\tau, j \mid \vec{n}, t)}{\sum_j p(\tau, j \mid \vec{n}, t)} = \text{prob. this is reaction } j = \frac{w_j(\bar{n})}{w_0(\bar{n})} .$$

Then we have the following algorithm:

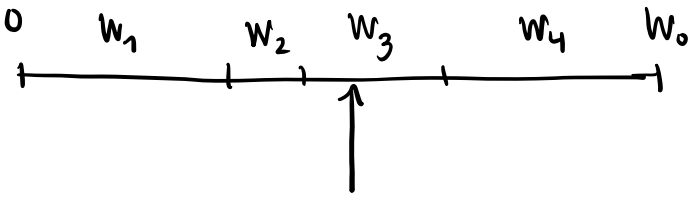
(0). Set initial conditions, $\vec{n} = \bar{n}_0$.

(1). Evaluate $w_j(\bar{n})$ for each possible reaction. Compute $w_0(\bar{n}) \equiv \sum_j w_j(\bar{n})$.

(2) Sample next reaction time from an exp. distrib. by mean $w_0(\bar{n})$.

(3) Choose which reaction occurs with uniform

probs. w_j / w_0 :



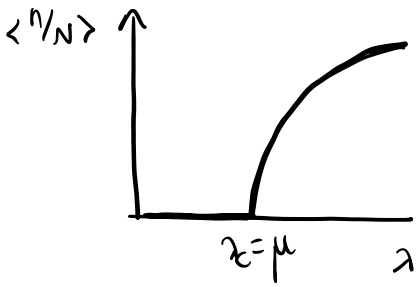
u = uniform random number in $[0, w_0]$. In this case, reaction 3 will take place.

(4.) Update the state of the system accordingly. Go to step 1.

PRACTICE

* Generate 5 trajectories of the SIS model with $\mu = 1$, $\lambda = 2$, $N = 1000$. Set initial condition $n_I = n_S = N/2$.

** setting $\mu = 1$, $N = 1000$, plot $\langle n/N \rangle$ evaluated at stationarity as a function of λ. You should see a sort of phase transition.



(I will appear "noisy")