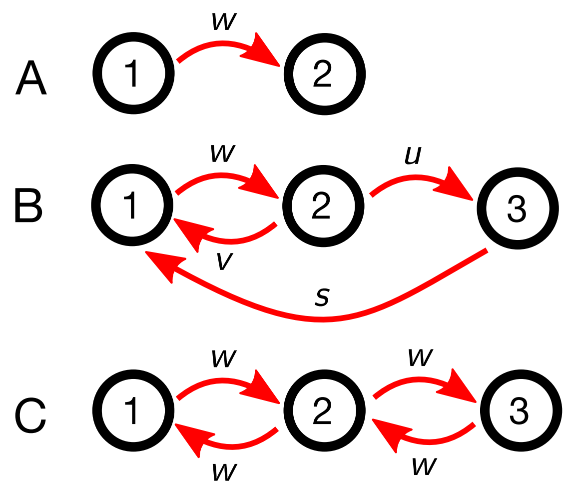
PHYS 320: Mastering the master equation
Part I: Writing it down



The master equation allows us to describe stochastic dynamics in a wide variety of biological models. The starting point for constructing this equation is always to identify the relevant states of the system, and the transition rates between them. Consider the three simple examples on the right, where the black circles denote the states and the red arrows the allowed transitions.

Let us start our discussion with system A, which is the simplest stochastic model one can construct. The red arrow labeled w means that *if* the system is in state 1 at any time t, the probability of jumping to state 2 between time t and $t + \delta t$ is $w\delta t$. Note the emphasis on the word *if*: the probability $w\delta t$ is conditioned on the assumption you are in state 1 at time t. But we are not necessarily in state 1 at time t. Imagine we are running many experimental trials, all initiated in state 1 at $t = 0$, which corresponds to having probability $p_1(0) = 1$. If we watch our experiments until time t, some of them will remain in state 1 (a fraction $p_1(t)$ of the total), while the remainder (a fraction $p_2(t) = 1 - p_1(t)$) will now be in state 2.

Thus the probability of seeing a jump from 1 to 2 between times t and $t + \delta t$ is actually $wp_1(t)\delta t$. This is because for the jump to happen, two conditions must be fulfilled: you have to be in state 1 (probability $p_1(t)$) and a jump must occur from 1 to 2 (probability $w\delta t$). The probability of observing the jump is the product of these two probabilities. Multiplying by $p_1(t)$ is important: for example if $p_1(t) = 0$ (none of the experimental systems were in state 1 at time t) then you would not see any jumps from 1 to 2 between t and $t + \delta t$.

Transition rates: In general, let $\Omega_{ii'}\delta t$ be the probability that *if* the system is in state i' at time t, a jump to different state $i \neq i'$ will occur in the time interval t to $t+\delta t$. The probability of actually seeing such a jump is $\Omega_{ii'}p_{i'}(t)\delta t$. If there are N states, the values $\Omega_{ii'}$ are called *transition rates*, and the Ω is the transition rate matrix. (We will define the diagonal elements of this matrix later.) Graphically, $\Omega_{ii'}$ is a red arrow from i' to i, and $p_{i'}(t)$ is the probability of the state where the arrow originates.

Returning to system A, we can now write down dynamical equations for $p_1(t)$ and $p_2(t)$. The fraction of experimental trials in state 1 at time $t + \delta t$ can be broken down as follows:

$$\begin{aligned}(\text{fraction of trials in state 1 at time } t+\delta t) &= (\text{fraction of trials in state 1 at time } t)\\ &\quad - (\text{fraction of trials where a jump 1 to 2}\\ &\qquad \text{was observed between } t \text{ and } t+\delta t)\end{aligned}$$

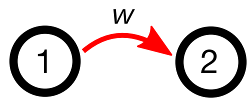
In probability terms, this translates to:

$$p_1(t+\delta t) = p_1(t) - wp_1(t)\delta t$$

Since each observed jump $1 \to 2$ adds to the fraction in state 2, we have the following equation for state 2:

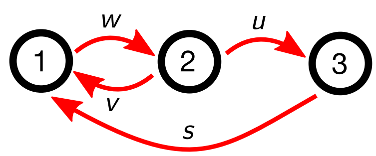
$$p_2(t + \delta t) = p_2(t) + wp_1(t)\delta t$$

Dividing through by δt and taking the limit $\delta t \to 0$, we can rewrite these equations as:



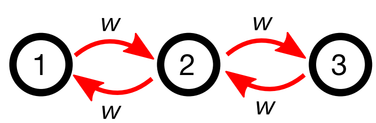
$$\begin{aligned}\frac{dp_1}{dt} &= -wp_1, \\ \frac{dp_2}{dt} &= wp_1\end{aligned} \tag{1}$$

For any system, the right-hand side of the master equation for state i is always the sum of contributions from each arrow going into or out of state i, giving positive or negative terms respectively. For example, convince yourself that the following equations describe System B, which has three states:



$$\begin{aligned}\frac{dp_1}{dt} &= -wp_1 + vp_2 + sp_3, \\ \frac{dp_2}{dt} &= wp_1 - (u + v)p_2, \\ \frac{dp_3}{dt} &= up_2 - sp_3\end{aligned} \tag{2}$$

Finally, here are the equations for system C, which is a three-state version of our diffusion model along one coordinate,



$$\begin{aligned}\frac{dp_1}{dt} &= -wp_1 + wp_2, \\ \frac{dp_2}{dt} &= wp_1 - 2wp_2 + wp_3, \\ \frac{dp_3}{dt} &= wp_2 - wp_3\end{aligned} \tag{3}$$

General master equation: The right-hand side of the equation for dp_i/dt for a given state i is a sum of two types of contributions: a) arrows going into i from $i' \neq i$, each giving a positive factor of $\Omega_{ii'}p_{i'}$; b) arrows going out of i to some $i' \neq i$, each giving a factor of $-\Omega_{i'i}p_i$. The net result is an equation:

$$\frac{dp_i}{dt} = \sum_{i' \neq i} \Omega_{ii'}p_{i'} - \sum_{i' \neq i} \Omega_{i'i}p_i \tag{4}$$

To write this as a matrix-vector product on the right-hand side, we define the diagonal elements of the matrix Ω as:

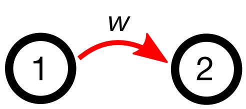
$$\Omega_{ii} \equiv -\sum_{i' \neq i} \Omega_{i'i}$$

Note that this is the same as saying that each column of Ω always adds up to zero. As we saw in class, this guarantees that the probability $p_i(t)$ which is a solution to the master equation is always normalized. Physically, the absolute value $|\Omega_{ii}|$ is the total transition rate for leaving state i, summing all possible jumps to other states $i' \neq i$.

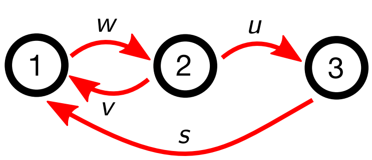
With the above definition of Ω_{ii}, Eq. (4) becomes:

$$\begin{aligned} \frac{dp_i}{dt} &= \sum_{i' \neq i} \Omega_{ii'} p_{i'} + \Omega_{ii} p_i \\ &= \sum_{i'} \Omega_{ii'} p_{i'} \\ \Rightarrow \qquad \frac{d\mathbf{p}}{dt} &= \Omega \mathbf{p}, \end{aligned} \tag{5}$$

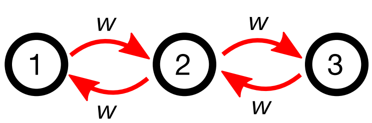
where $\mathbf{p}(t)$ is the vector with components $p_i(t)$. The matrix-vector forms of the three master equations above, Eqs. (1)-(3), are:



$$\frac{d}{dt}\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} -w & 0 \\ w & 0 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$$



$$\frac{d}{dt}\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -w & v & s \\ w & -(u+v) & 0 \\ 0 & u & -s \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \tag{6}$$



$$\frac{d}{dt}\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -w & w & 0 \\ w & -2w & w \\ 0 & w & -w \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$