Notes on Master Equation Methods

1   Transition and Other Matrices

Standard master equation has the form of

$$\partial_t p_i = \sum_j \left(R_{ij} p_j - R_{ji} p_i \right) \tag{1}$$

where R_{ij} corresponds to the $j \to i$ transition. For a steady state we must have $\partial_t p_i = 0$ and if each term in the sum of eq. (1) is independently 0 we have detailed balance. In general however to solve for 0 it is convenient to put the equation in a eigenvalue like form such as

$$\partial_t p_i = \sum_j W_{ij} p_j \tag{2}$$

for some matrix $\underline{\underline{W}}$. This matrix can be expressed in terms of $\underline{\underline{R}}$ as

$$W_{ij} = R_{ij} - \delta_{ij} \sum_k R_{ki} \tag{3}$$

as this leads to

$$\partial_t p_i = \sum_j W_{ij} p_j = \sum_j \left(R_{ij} - \delta_{ij} \sum_k R_{ki} \right) p_j = \tag{4}$$

$$= \sum_j R_{ij} p_j - \sum_{j,k} \delta_{ij} R_{ki} p_j = \tag{5}$$

$$= \sum_j R_{ij} p_j - \sum_k R_{ki} p_i = \tag{6}$$

$$= \sum_j \left(R_{ij} p_j - R_{ji} p_i \right) \quad \text{as required} \tag{7}$$

2   Eigensystem of $\underline{\underline{W}}$

Without proof, such a matrix will always have 0 as an eigenvalue. If the matrix/system is connected this will be associated with one eigenstate. Further, all other eigenvalues have negative real parts and their eigenstates' components sum to 0.

From eq. (2) it's clear that the eigenstate(s) with 0 eigenvalue form the steady state (or space). The others are not so clear, consider having at $t = 0$ a state $\underline{p}(0) = \underline{p}_0 + \underline{\delta}$ with $\underline{p}_0$ being a steady state. Then we will have

$$\partial_t \underline{p} \Big|_{t=0} = \underline{\underline{W}} \cdot \underline{\delta} \quad \text{so that} \quad \underline{p}(\delta t) = \underline{p}(0) + \delta t \underline{\underline{W}} \cdot \underline{\delta} = \underline{p}_0 + \left(\underline{\underline{1}} + \delta t \underline{\underline{W}} \right) \cdot \underline{\delta} \tag{8}$$

This gets particularly interesting when $\underline{\delta}$ is itself an eigenvalue of $\underline{\underline{W}}$. If $\underline{\underline{W}} \cdot \underline{\delta} = \lambda \underline{\delta}$ then

$$\partial_t \underline{p} \Big|_{t=0} = \lambda \underline{\delta} \quad \text{and} \quad \underline{p}(\delta t) = \underline{p}_0 + (1 + \delta t \lambda) \underline{\delta} \tag{9}$$

which notably is of the same form as $\underline{p}(0)$ just with a rescaled $\underline{\delta}$. Thus we can conclude that for any such starting state we have $\underline{p}(t) = \underline{p}_0 + a(t) \underline{\delta}$ for some function $a(t)$. Notably here $\underline{p}_0$ and $\underline{\delta}$ do not have to be mutually orthogonal, if they are not than this is not the only way of writing the functional form of $\underline{p}(t)$ but it is still a valid one.

This then leads to

$$\underline{p}(t + \delta t) = \underline{p}_0 + a(t + \delta t) \underline{\delta} = \underline{p}(t) + \delta t \frac{\partial \underline{p}}{\partial t} \Big|_t = \underline{p}_0 + a(t) \underline{\delta} + \delta t \lambda a(t) \underline{\delta} \tag{10}$$

after eliminating $\underline{p}_0$ we get

$$a(t + \delta t) \underline{\delta} = a(t) \underline{\delta} + \delta t \lambda a(t) \underline{\delta} \implies \tag{11}$$

$$\frac{a(t + \delta t) - a(t)}{\delta t} = \lambda a(t) \tag{12}$$

giving the predictable result of $a(t) = a(0) e^{\lambda t}$.

> So in summary, any non-steady eigenstate $\underline{\delta}$ of $\underline{\underline{W}}$ can be seen as a perturbation mode which if superposed over a steady state will decay exponentially with its associated eigenvalue as $e^{\lambda t}$. Naturally if there are degenerate eigenstates with the same eigenvalue we get a perturbation space for that eigenvalue.

though there remains the question of complex eigenvalues and eigenstates. It seems natural that imaginary components of eigenvalues would correspond to oscillations and I mostly just hope that eigenstates do not have imaginary components

3   Gillespie Simulations

Going off of the 2007 paper by Gillespie: `https://www.annualreviews.org/content/journals/10.1146/annurev.physchem.58.032806.104637`. Alogirthm for realizing trajectories starts above equation 7.

Okay so from what I understand, the algorithm to choose the time and type of process out of a known set of processes each with its rate r_i is as follows. Choose a random process with the probability of getting each of proportional to it's rate (in other words equal to $\frac{r_i}{r_0}$). Then choose a random number from an exponential distribution of $\text{pdf}(x) = e^{-r_0 x}$ with $r_0 = \sum_j r_j$ and we have τ equal to r_i times the random number.