The Finite State Projection Algorithm

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September 9, 2022

Master equations

- Master equations describe the time-evolution of a discrete state Markov process in continous time
- We define a probability T_{ij} of transitioning to the arbitrary state ω_j from ω_i where $\omega_i, \omega_j \in \Omega$
- These probabilities are efficiently described by a matrix $\mathbf{T} \in \mathbb{R}^{N \times N}$ where $N = |\Omega|$
- $\mathbf{T}[(I, t + dt), (j, t)] = \mathbf{Pr}\left((I, t + dt), (j, t)\right)$ is a conditional distribution, given that we are in a state j at time t

Initially we assume $\boldsymbol{T}$ is constant in time

The forward equation

The time evolution of $P(\Omega, t) \in \mathbb{R}^{N\times 1}$ is determined by the net probability flux into and out of each state:

$$P(\omega_i, t+dt) = \overbrace{T_{ii}P(\omega_i)dt + \sum_{j\neq i} T_{ij}P(\omega_j, t)dt}^{j\rightarrow i} + \overbrace{\sum_{j\neq i} T_{ji}P(\omega_i, t)dt}^{i\rightarrow j}$$

$$= \overbrace{\sum_{j\neq i} T_{ij}P(\omega_j, t)dt}^{j\rightarrow i} + \overbrace{P(\omega_i, t)\sum_{j} T_{ji}dt}^{i\rightarrow j}$$

$$= \overbrace{\sum_{j\neq i} T_{ij}P(\omega_j, t)dt}^{j\rightarrow i} + \overbrace{P(\omega_i, t)\left(1 - \sum_{j} T_{ij}dt\right)}^{i\rightarrow j}$$

$$P(\omega_i, t + dt) = \sum_{j \neq i} T_{ij} P(\omega_j, t) dt + P(\omega_i, t) \left(1 - \sum_j T_{ij} dt \right)$$

$$\lim_{dt \to 0} \frac{P(\omega_i, t + dt) - P(\omega_i, t)}{dt} = \sum_{j \neq i} T_{ij} P(\omega_j, t) - P(\omega_i, t) \sum_j T_{ij}$$

Rearranging, we arrive at the **master equation**

$$\frac{dP(\omega_i)}{dt} = \sum_j T_{ji} P(\omega_j, t) - T_{ij} P(\omega_i, t)$$

Operator formulation

It is common to then define an operator $\boldsymbol{W}$ s.t. $W_{ij} = T_{ij}$ and $W_{ii} = -\sum_j T_{ij}$

$$\frac{dP(\omega_i)}{dt} = \sum_j W_{ij} P(\omega_j) \rightarrow \frac{dP(\omega)}{dt} = \mathbf{W} P(\omega)$$

We have the following simplified form of a general master equation

$$\frac{dP(\omega)}{dt} = \mathbf{W} P(\omega)$$

The chemical master equation

We transition from a state ω_j to ω_i via reaction $\boldsymbol{\nu}$

Thus states are related by $\omega_i = \omega_j + \boldsymbol{\nu}_j$. Suppose that $\boldsymbol{T}$ varies with the state $\boldsymbol{x}$

$$\begin{aligned}\frac{dP(\omega_i)}{dt} &= \sum_j T_{ji} P(\omega_j, t) - T_{ij} P(\omega_i, t) \\ &= \sum_j T_{ji}(\boldsymbol{x} - \boldsymbol{\nu}) P_j(\boldsymbol{x} - \boldsymbol{\nu}, t) - T_{ij}(\boldsymbol{x}) P_j(\boldsymbol{x}, t)\end{aligned}$$

Or in vector form, we have

$$\frac{dP(\boldsymbol{x})}{dt} = \sum_j T_j(\boldsymbol{x} - \boldsymbol{\nu}) P_j(\boldsymbol{x} - \boldsymbol{\nu}, t) - T_j(\boldsymbol{x}) P_j(\boldsymbol{x}, t)$$

The chemical master equation intuition

We arrived at the following equation

$$\mathcal{J} = \frac{dP(\boldsymbol{x})}{dt} = \sum_j T_j(\boldsymbol{x} - \boldsymbol{\nu})P_j(\boldsymbol{x} - \boldsymbol{\nu}, t) - T_j(\boldsymbol{x})P_j(\boldsymbol{x}, t)$$

where $\mathcal{J}$ is a probability current

$P(\boldsymbol{x}, t)$ is a density over the state space Ω. This is then a sum over the entire state space

Each term of the above sum is a vector multiplied by a scalar. The current $\mathcal{J}$ is a vector expressed as a sum of vectors

The chemical master equation intuition

We write it as a matrix multiplication by arranging $T_j(\boldsymbol{x} - \boldsymbol{\nu}_j)$ as the columns of a matrix $\mathcal{L}(\boldsymbol{x} - \boldsymbol{\nu}_j)$

$$\mathcal{J}(\mathbf{x}, t) = \mathcal{L}(\boldsymbol{x} - \boldsymbol{\nu}_j, t)P(\boldsymbol{x} - \boldsymbol{\nu}_j, t) - \mathcal{L}(\boldsymbol{x}, t)P(\boldsymbol{x}, t)$$

But $\boldsymbol{\nu}_i = 0$ so we define $\mathbf{W} = \mathcal{L}(\boldsymbol{x} - \boldsymbol{\nu}_j, t) - \mathrm{diag}\left(\mathcal{L}(\boldsymbol{x}, t)\right)$ which gives

$$\mathcal{J}(\mathbf{x}, t) = \mathbf{W}P(\boldsymbol{x}, t)$$