S5.D. Approximations to the Master Equation

For certain types of transition rates w_{mn}, the master equation

$$\frac{\partial P(n,t)}{\partial t} = \sum_{m=1}^{M} \left[P(m,t)\, w_{mn}(t) - P(n,t)\, w_{nm}(t) \right] \tag{5.53}$$

can be reduced to a Fokker-Planck equation as the realizations y_n of the stochastic variable Y becomes continuous, i.e.,

$$\Delta y_n = y_n - y_{n-1} \to 0$$

Reminder: $P(n, t)$ is the shorthand for $P(y_n, t)$.

As an example, consider the 1-D random walk of step size Δ. The distance X from the starting point is the stochastic variable with realizations $x_n = n\,\Delta$, which becomes a continuous variable x as $\Delta \to 0$. If the transition rates are time independent but depend on Δ, (5.53) can be written as

$$\frac{\partial P(n\Delta,t)}{\partial t} = \sum_{m=-\infty}^{\infty} \left[P(m\Delta,t)\, w_{mn}(\Delta) - P(n\Delta,t)\, w_{nm}(\Delta) \right] \tag{5.158}$$

If we choose

$$w_{mn}(\Delta) = \frac{1}{\Delta^2} \left(\delta_{m,n+1} + \delta_{m,n-1} \right) \tag{5.159}$$

then (5.158) becomes

$$\begin{aligned} \frac{\partial P(n\Delta,t)}{\partial t} &= \frac{1}{\Delta^2} \sum_{m=-\infty}^{\infty} \Big[P(m\Delta,t)\, (\delta_{m,n+1} + \delta_{m,n-1}) \\ &\qquad\qquad - P(n\Delta,t)\, (\delta_{n,m+1} + \delta_{n,m-1}) \Big] \\ &= \frac{1}{\Delta^2} \left\{ P\big[(n+1)\Delta, t\big] + P\big[(n-1)\Delta, t\big] - 2\,P(n\Delta,t) \right\} \end{aligned} \tag{5.160}$$

As $\Delta \to 0$, this becomes

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial^2 P(x,t)}{\partial x^2} \tag{5.161}$$

which is the Fokker-Planck equation for a free Brownian particle [c.f. (5.144)].

A more general result can be obtained starting with the master equation for a stochastic variable with continuous realization,

$$\frac{\partial P(x,t)}{\partial t} = \int_{-\infty}^{\infty} d\,x' \left[P(x',t)\, w(x' \mid x) - P(x,t)\, w(x \mid x') \right] \tag{5.162}$$

where, for convenience, we assume the transition rates to be time-independent.

Setting

$$x' = x + y$$

(5.162) becomes

$$\frac{\partial P(x,t)}{\partial t} = \int_{-\infty}^{\infty} d\,y \left[P(x+y,t)\, w(x+y \mid x) - P(x,t)\, w(x \mid x+y) \right] \tag{5.162a}$$

Let

$$\tau(x,y) = w(x \mid x+y) \qquad \xrightarrow{x \to x-y} \qquad \tau(x-y,y) = w(x-y \mid x) \tag{5.162b}$$

Setting $y \to -y$ in the 1st integral in (5.162a) gives

$$\frac{\partial P(x,t)}{\partial t} = \int_{-\infty}^{\infty} dy \left[P(x-y,t)\; w(x-y \mid x) - P(x,t)\, w(x \mid x+y) \right]$$

$$= \int_{-\infty}^{\infty} dy \left[P(x-y,t)\; \tau(x-y,y) - P(x,t)\, \tau(x,y) \right] \qquad \text{[(5.162b) used.]}$$

$$= \int_{-\infty}^{\infty} dy \left[\sum_{n=0}^{\infty} \frac{(-y)^n}{n!} \frac{\partial^n P(x,t)\; \tau(x,y)}{\partial x^n} - P(x,t)\, \tau(x,y) \right] \qquad \text{[Taylor Series]}$$

$$= \int_{-\infty}^{\infty} dy \sum_{n=1}^{\infty} \frac{(-y)^n}{n!} \frac{\partial^n P(x,t)\; \tau(x,y)}{\partial x^n} \qquad (5.164)$$

$$= \sum_{n=1}^{\infty} \frac{(-)^n}{n!} \frac{\partial^n}{\partial x^n} \left[P(x,t) \int_{-\infty}^{\infty} dy\; y^n\, \tau(x,y) \right]$$

$$= \sum_{n=1}^{\infty} \frac{(-)^n}{n!} \frac{\partial^n}{\partial x^n} \left[P(x,t)\, \alpha_n(x) \right] \qquad (5.165)$$

where

$$\alpha_n(x) = \int_{-\infty}^{\infty} dy\; y^n\, \tau(x,y)$$

$$= \int_{-\infty}^{\infty} dy\; y^n\; w(x \mid x+y) \qquad (5.166)$$

(5.165) is known as the Kramers-Moyal expansion of the master equation. Obviously, it is useful only if the series terminates after a few terms.

For example, let

$$w(x \mid x+y) = \tau(x,y) = \frac{1}{\sqrt{\pi}\, \Delta^3} \exp\left(-\frac{\left(y - A(x)\, \Delta^2\right)^2}{\Delta^2} \right) \qquad (5.167)$$

Using *Mathematica* to calculate the Gaussian integrals, we have [see §Code],

$$\alpha_0 = \int_{-\infty}^{\infty} dy\, w(x \mid x+y) = \frac{1}{\Delta^2} \qquad \text{[c.f. (5.159)]}$$

$$\alpha_1 = A$$

$$\alpha_2 = \frac{1}{2} + A^2\, \Delta^2$$

and for $n \geq 1$,

$$\alpha_{2n+1} = O\left(\Delta^{2n}\right)$$

$$\alpha_{2n+2} = O\left(\Delta^{2n}\right)$$

Thus, for $\Delta \to 0$, only α_1 and α_2 contribute to the Kramers-Moyal equation (5.165), giving

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}[A(x)\, P(x,t)] + \frac{1}{4} \frac{\partial^2}{\partial x^2} P(x,t) \qquad (5.170)$$

In cases like chemical reactions or population dynamics, $\Delta \to 0$ is not valid. The Kramers-Moyal expansion is then invalid and the master equation must be solved by other means, e.g., numerically. An alternative approximation scheme introduced by van Kampen can be found in his book, “Stochastic Processes in Physics & Chemistry”, North Holland (1992).

Code

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(* α_{2n+1} *)
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$$\text{Assuming}\left[(n \in \text{Integers} \;\&\&\; n \geq 0) \;\&\&\; a \geq 0 \;\&\&\; \Delta > 0,\ \frac{1}{\sqrt{\pi}\,\Delta^3}\int_{-\infty}^{\infty}\text{Exp}\left[-\frac{(y - A\,\Delta^2)^2}{\Delta^2}\right] y^{2n+1}\, dy\right]$$

$$\frac{2\,A\,\Delta^{2n}\,\text{Gamma}\left[\frac{3}{2}+n\right]\,\text{Hypergeometric1F1}\left[-n,\ \frac{3}{2},\ -A^2\,\Delta^2\right]}{\sqrt{\pi}}$$

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(* α_{2n} *)
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$$\text{Assuming}\left[(n \in \text{Integers} \;\&\&\; n \geq 0) \;\&\&\; a \geq 0 \;\&\&\; \Delta > 0,\ \frac{1}{\sqrt{\pi}\,\Delta^3}\int_{-\infty}^{\infty}\text{Exp}\left[-\frac{(y - A\,\Delta^2)^2}{\Delta^2}\right] y^{2n}\, dy\right]$$

$$\frac{\Delta^{-2+2n}\,\text{Gamma}\left[\frac{1}{2}+n\right]\,\text{Hypergeometric1F1}\left[-n,\ \frac{1}{2},\ -A^2\,\Delta^2\right]}{\sqrt{\pi}}$$

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(* α_0, α_2, α_4, α_6, α_8, α_10 *)
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$$\text{Table}\left[\text{Assuming}\left[a \geq 0 \;\&\&\; \Delta > 0,\ \frac{1}{\sqrt{\pi}\,\Delta^3}\int_{-\infty}^{\infty}\text{Exp}\left[-\frac{(y - A\,\Delta^2)^2}{\Delta^2}\right] y^{2n}\, dy\right],\ \{n,\ 0,\ 5\}\right]$$

$$\left\{\frac{1}{\Delta^2},\ \frac{1}{2}\left(1+2\,A^2\,\Delta^2\right),\ \frac{1}{4}\,\Delta^2\left(3+12\,A^2\,\Delta^2+4\,A^4\,\Delta^4\right),\right.$$
$$\frac{1}{8}\,\Delta^4\left(15+90\,A^2\,\Delta^2+60\,A^4\,\Delta^4+8\,A^6\,\Delta^6\right),\ \frac{1}{16}\,\Delta^6\left(105+840\,A^2\,\Delta^2+840\,A^4\,\Delta^4+224\,A^6\,\Delta^6+16\,A^8\,\Delta^8\right),$$
$$\left.\frac{1}{32}\,\Delta^8\left(945+2\,A^2\,\Delta^2\left(4725+4\,A^2\,\Delta^2\left(1575+630\,A^2\,\Delta^2+90\,A^4\,\Delta^4+4\,A^6\,\Delta^6\right)\right)\right)\right\}$$

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(* α_1, α_3, α_5, α_7, α_9, α_11 *)
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$$\text{Table}\left[\text{Assuming}\left[a \geq 0 \;\&\&\; \Delta > 0,\ \frac{1}{\sqrt{\pi}\,\Delta^3}\int_{-\infty}^{\infty}\text{Exp}\left[-\frac{(y - A\,\Delta^2)^2}{\Delta^2}\right] y^{2n+1}\, dy\right],\ \{n,\ 0,\ 5\}\right]$$

$$\left\{A,\ \frac{1}{2}\,A\,\Delta^2\left(3+2\,A^2\,\Delta^2\right),\ \frac{1}{4}\,A\,\Delta^4\left(15+20\,A^2\,\Delta^2+4\,A^4\,\Delta^4\right),\ \frac{1}{8}\,A\,\Delta^6\left(105+210\,A^2\,\Delta^2+84\,A^4\,\Delta^4+8\,A^6\,\Delta^6\right),\right.$$
$$\frac{1}{16}\,A\,\Delta^8\left(945+8\,A^2\,\Delta^2\left(315+189\,A^2\,\Delta^2+36\,A^4\,\Delta^4+2\,A^6\,\Delta^6\right)\right),$$
$$\left.\frac{1}{32}\,A\,\Delta^{10}\left(10\,395+2\,A^2\,\Delta^2\left(17\,325+4\,A^2\,\Delta^2\left(3465+990\,A^2\,\Delta^2+110\,A^4\,\Delta^4+4\,A^6\,\Delta^6\right)\right)\right)\right\}$$