1 General Fokker-Planck Equation

Consider a process that is described by nonlinear Langevin equations (using Einstein's summation convention)

$$\dot{\zeta}_i = h_i\left(\{\zeta\}, t\right) + g_{ij}\left(\{\zeta\}, t\right)\Gamma_j\left(t\right), \tag{1}$$

where $\{\zeta\} = \zeta_1, \zeta_2, \ldots \zeta_N$.

Typically, a general formal solution to (1) cannot be obtained. However, one may derive a Fokker-Planck equation which allows for the calculation of the probability density of the stochastic variable. The Fokker-Planck equation follows from the Kramers-Moyal forward expansion of the distribution function $W\left(\{x\}, t\right)$ (Risken, 63–66, 81–82):

$$\frac{\partial W\left(\{x\}, t\right)}{\partial t} = \sum_{\nu=1}^{\infty} \frac{\left(-\partial\right)^{\nu}}{\partial x_{j_1}\cdots\partial x_{j_\nu}} D^{(\nu)}_{j_1,\ldots,j_\nu}\left(\{x\}, t\right) W\left(\{x\}, t\right), \tag{2}$$

where the Kramers-Moyal coefficients are defined by (Risken, 56)

$$D^{(\nu)}_{i_1,\ldots,i_\nu}\left(\{x\}, t\right) = \frac{1}{\nu!}\lim_{\tau\to 0}\frac{1}{\tau}\langle[\zeta_{i_1}\left(t+\tau\right) - x_{i_1}]\cdots[\zeta_{i_\nu}\left(t+\tau\right) - x_{i_\nu}]\rangle. \tag{3}$$

The solution of (2) with the initial condition

$$W\left(\left\{x'\right\}, t'\right) = P\left(\{x\}, t' \mid \left\{x'\right\}, t'\right) = \delta\left(\{x\} - \left\{x'\right\}\right)$$

is the transition probability P. So, the forward equation for the probability density is given by

$$\frac{\partial P\left(\{x\}, t \mid \{x'\}, t'\right)}{\partial t} = \mathbf{L}_{\mathrm{KM}} P\left(x, t \mid \left\{x'\right\}, t'\right), \tag{4}$$

where $\mathbf{L}_{\mathrm{KM}}$ denotes the Kramers-Moyal differential operator

$$\mathbf{L}_{\mathrm{KM}} = \sum_{\nu=1}^{\infty} \frac{\left(-\partial\right)^{\nu}}{\partial x_{j_1}\cdots\partial x_{j_\nu}} D^{(\nu)}_{j_1,\ldots,j_\nu}\left(\{x\}, t\right).$$

If the Langevin forces in (1) are δ-correlated Gaussian random variables, that is, Γ_i satisfy

$$\langle\Gamma_i\left(t\right)\rangle = 0, \qquad \langle\Gamma_i\left(t\right)\Gamma_j\left(t'\right)\rangle = 2\delta_{ij}\delta\left(t - t'\right), \tag{5}$$

then $D^{(\nu)}_{i_1,\ldots,i_\nu}\left(\{x\}, t\right) = 0$ for $\nu \geq 3$ (Risken, 56, 83). As a result, we obtain the Fokker-Planck equation for the transition probability:

$$\frac{\partial P\left(\{x\}, t \mid \{x'\}, t'\right)}{\partial t} = \mathbf{L}_{\mathrm{FP}} P\left(x, t \mid \left\{x'\right\}, t'\right), \tag{6}$$

$$\mathbf{L}_{\mathrm{FP}} = -\frac{\partial}{\partial x_i} D_i\left(\{x\}, t\right) + \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}\left(\{x\}, t\right), \tag{7}$$

with initial condition

$$P\left(\{x\}, t' \mid \left\{x'\right\}, t'\right) = \delta\left(\{x\} - \left\{x'\right\}\right). \tag{8}$$

The coefficients D_i and D_{ij} in (6) are called the drift vector and diffusion matrix, respectively, and can be shown to satisfy (Risken, 55)

$$D_i(\{x\},t) = h_i(\{x\},t) + g_{kj}(\{x\},t)\frac{\partial}{\partial x_k}g_{ij}(\{x\},t), \tag{9}$$

$$D_{ij}(\{x\},t) = g_{ik}(\{x\},t)\,g_{jk}(\{x\},t). \tag{10}$$

Note that the diffusion matrix can be shown to be symmetric, semidefinite, and singular (Risken, 84, 87).

If we multiply (6) by $W(\{x'\},t')$ and integrate over $\{x'\}$, we obtain the Fokker-Planck equation for the probability density $W(\{x\},t)$:

$$\frac{\partial W(\{x\},t)}{\partial t} = \mathbf{L}_{\mathrm{FP}}W(x,t) \tag{11}$$

This equation can then be rewritten in the form of the continuity equation

$$\frac{\partial W}{\partial t} + \frac{\partial S_i}{\partial x_i} = 0, \tag{12}$$

where the probability current S_i is defined by (Risken, 84)

$$S_i = D_i W - \left(\frac{\partial}{\partial x_j}\right) D_{ij} W. \tag{13}$$

2 Kramers Equation

The Langevin equation describing the Brownian motion of particles with mass m in a potential $mf(x)$ is given by

$$m\ddot{x} + m\gamma\dot{x} + mf'(x) = m\Gamma(t), \tag{14}$$

$$\langle\Gamma(t)\rangle = 0, \qquad \langle\Gamma(t)\,\Gamma(t')\rangle = 2\gamma\,(kT/m)\,\delta\left(t-t'\right), \tag{15}$$

where Γ is Gaussian distributed, γ is the damping constant, $-f'(x)$ is the force per mass m due to the potential $mf(x)$, k is Boltzmann's constant, and T is the temperature of the surrounding heat bath. The corresponding Fokker-Planck equation is called the Kramers equation and is obtained by first writing (14) as a system of two first-order equations

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= -\gamma v - f'(x) + \Gamma(t). \end{aligned} \tag{16}$$

Then, from (6)–(10,) the Kramers equation is given by

$$\frac{\partial P(x,v,t \mid x',v',0)}{\partial t} = \mathbf{L}_{\mathrm{K}}P\left(x,v,t \mid x',v',0\right), \tag{17}$$

$$\mathbf{L}_{\mathrm{K}} = \mathbf{L}_{\mathrm{K}}(x,v) = -\frac{\partial}{\partial x}v + \frac{\partial}{\partial v}\left[\gamma v + f'(x)\right] + \gamma v_{th}^2\frac{\partial^2}{\partial v^2}, \tag{18}$$

where $P(x,v,t \mid x',v',0)$ is the transition probability in position and velocity space with $0 \le x \le L, -\infty < v < \infty$, and $t \ge 0$, and $v_{th}^2 = \sqrt{kT/m}$ is the thermal velocity.

2.1 Initial and Boundary Conditions

The initial condition for P in (17) is given by

$$P\left(x, v, t \mid x', v', 0\right) = \delta\left(x - x'\right)\delta\left(v - v'\right). \tag{19}$$

Note that if the particles are injected at x' with a velocity distribution $g\left(v\right)$, then the δ-function above is replaced by $g\left(v\right)$.

With regard to boundary conditions, there are essentially two types to consider: reflecting and absorbing. Particles that hit a reflecting boundary with, say, velocity v are redirected with velocity $-v$. On the other hand, a particle hitting an absorbing boundary for the first time will be immediately removed from the interval. Assuming that we have a reflecting boundary at $x = 0$ and an absorbing boundary at $x = L$, we therefore obtain

$$\begin{aligned} P\left(0, v, t \mid x', v', 0\right) &= P\left(0, -v, t \mid x', v', 0\right), \\ P\left(L, v, t \mid x', v', 0\right) &= 0, \qquad v < 0. \end{aligned} \tag{20}$$

2.2 Steady State Solution

The steady state solution to (17)–(20) is given by the Boltzmann distribution

$$B(x, v) = N \exp\left[-E/(kT)\right], \tag{21}$$

where $E = mv^2/2 + mf(x)$. and N is an appropriately chosen normalization constant (Risken, 8). To see this, observe first that $B(x, v) = N\phi(x)\psi(v)$, where $\phi(x) = \exp\left[-mf(x)/(kT)\right]$ and $\psi(v) = \exp\left[-mv^2/(2kT)\right]$. So,

$$\begin{aligned} \phi'(x) &= \frac{-mf'(x)}{kT}\exp\left[-mf(x)/(kT)\right] = \frac{-mf'(x)}{kT}\phi(x), \\ \psi'(v) &= \frac{-mv}{kT}\exp\left[-mv^2/(kT)\right] = \frac{-mv}{kT}\psi(v), \\ \psi''(v) &= \frac{-m}{kT}\psi(v) + \frac{-mv}{kT}\psi'(v) = \left[\frac{m^2v^2}{k^2T^2} - \frac{m}{kT}\right]\psi(v), \end{aligned}$$

from which it follows

$$\begin{aligned} &-\frac{\partial}{\partial x}Bv = \frac{mf'(x)v}{kT}B, \\ &\frac{\partial}{\partial v}\left(\gamma v + f'(x)\right)B = \left[\gamma + \frac{-mv}{kT}\left(\gamma v + f'(x)\right)\right]B, \\ &\frac{\gamma kT}{m}\frac{\partial^2}{\partial v^2}B = \frac{\gamma kT}{m}\left[\frac{m^2v^2}{k^2T^2} - \frac{m}{kT}\right]B. \end{aligned}$$

Therefore,

$$\left[-\frac{\partial}{\partial x}v + \frac{\partial}{\partial v}\left(\gamma v + f'(x)\right) + \frac{\gamma kT}{m}\frac{\partial^2}{\partial v^2}\right]B(x, v) = 0$$

as required.