

1 General Fokker-Planck Equation

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

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

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

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 $W(\{x\}, t)$ (Risken, 63–66, 81–82):

$$\frac{\partial W(\{x\}, t)}{\partial t} = \sum_{\nu=1}^{\infty} \frac{(-\partial)^\nu}{\partial x_{j_1} \dots \partial x_{j_\nu}} D_{j_1, \dots, j_\nu}^{(\nu)}(\{x\}, t) W(\{x\}, t), \quad (2)$$

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

$$D_{i_1, \dots, i_\nu}^{(\nu)}(\{x\}, t) = \frac{1}{\nu!} \lim_{\tau \rightarrow 0} \frac{1}{\tau} \langle [\zeta_{i_1}(t + \tau) - x_{i_1}] \dots [\zeta_{i_\nu}(t + \tau) - x_{i_\nu}] \rangle. \quad (3)$$

The solution of (2) with the initial condition

$$W(\{x'\}, t') = P(\{x\}, t' | \{x'\}, t') = \delta(\{x\} - \{x'\})$$

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

$$\frac{\partial P(\{x\}, t | \{x'\}, t')}{\partial t} = \mathbf{L}_{\text{KM}} P(x, t | \{x'\}, t'), \quad (4)$$

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

$$\mathbf{L}_{\text{KM}} = \sum_{\nu=1}^{\infty} \frac{(-\partial)^\nu}{\partial x_{j_1} \dots \partial x_{j_\nu}} D_{j_1, \dots, j_\nu}^{(\nu)}(\{x\}, t).$$

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

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

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

$$\frac{\partial P(\{x\}, t | \{x'\}, t')}{\partial t} = \mathbf{L}_{\text{FP}} P(x, t | \{x'\}, t'), \quad (6)$$

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

with initial condition

$$P(\{x\}, t' | \{x'\}, t') = \delta(\{x\} - \{x'\}). \quad (8)$$

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)

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

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

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 $W(\{x\}, t)$:

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

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

$$\frac{\partial W}{\partial t} + \frac{\partial S_i}{\partial x_i} = 0, \quad (12)$$

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

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

2 Kramers Equation

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

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

$$\langle \Gamma(t) \rangle = 0, \quad \langle \Gamma(t) \Gamma(t') \rangle = 2\gamma(kT/m) \delta(t - t'), \quad (15)$$

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

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

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

$$\frac{\partial P(x, v, t \mid x', v', 0)}{\partial t} = \mathbf{L}_K P(x, v, t \mid x', v', 0), \quad (17)$$

$$\mathbf{L}_K = \mathbf{L}_K(x, v) = -\frac{\partial}{\partial x} v + \frac{\partial}{\partial v} [\gamma v + f'(x)] + \gamma v_{th}^2 \frac{\partial^2}{\partial v^2}, \quad (18)$$

where $P(x, v, t \mid x', v', 0)$ is the transition probability in position and velocity space with $0 \leq x \leq L$, $-\infty < v < \infty$, and $t \geq 0$, 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

$$P(x, v, t | x', v', 0) = \delta(x - x') \delta(v - v'). \quad (19)$$

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

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

$$\begin{aligned} P(0, v, t | x', v', 0) &= P(0, -v, t | x', v', 0), \\ P(L, v, t | x', v', 0) &= 0, \quad v < 0. \end{aligned} \quad (20)$$

2.2 Steady State Solution

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

$$B(x, v) = N \exp[-E/(kT)], \quad (21)$$

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 $\phi(x) = \exp[-mf(x)/(kT)]$ and $\psi(v) = \exp[-mv^2/(2kT)]$. So,

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

from which it follows

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

Therefore,

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

as required.