THE FOKKER-PLANCK EQUATION

Existence and Uniqueness of Solutions for the FP Equation

- Consider a diffusion process on $\mathbb{R}^d$ with time-independent drift and diffusion coefficients. The Fokker-Planck equation is

$$\frac{\partial p}{\partial t} = -\sum_{j=1}^{d} \frac{\partial}{\partial x_j}(a_i(x)p) + \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j}(b_{ij}(x)p), \; t > 0, \, x \in \mathbb{R}^d, \tag{1a}$$

$$p(x,0) = f(x), \quad x \in \mathbb{R}^d. \tag{1b}$$

- Write it in **non-divergence form**:

$$\frac{\partial p}{\partial t} = \sum_{j=1}^{d} \tilde{a}_j(x) \frac{\partial p}{\partial x_j} + \frac{1}{2}\sum_{i,j=1}^{d} \tilde{b}_{ij(x)} \frac{\partial^2 p}{\partial x_i \partial x_j} + \tilde{c}(x)u, \; t > 0, \, x \in \mathbb{R}^d, \tag{2a}$$

$$p(x,0) = f(x), \quad x \in \mathbb{R}^d, \tag{2b}$$

- where

$$\tilde{a}_i(x) = -a_i(x) + \sum_{j=1}^{d} \frac{\partial b_{ij}}{\partial x_j}, \quad \tilde{c}_i(x) = \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2 b_{ij}}{\partial x_i \partial x_j} - \sum_{i=1}^{d} \frac{\partial a_i}{\partial x_i}.$$

- The diffusion matrix is always nonnegative. We will assume that it is actually positive, i.e. we will impose the **uniform ellipticity** condition:

$$\sum_{i,j=1}^{d} b_{ij}(x)\xi_i\xi_j \geqslant \alpha \|\xi\|^2, \quad \forall \xi \in \mathbb{R}^d, \tag{3}$$

- Furthermore, we will assume that the coefficients $\tilde{a}$, b, $\tilde{c}$ are smooth and that they satisfy the growth conditions

$$\|b(x)\| \leqslant M, \ \|\tilde{a}(x)\| \leqslant M(1+\|x\|), \ \|\tilde{c}(x)\| \leqslant M(1+\|x\|^2). \tag{4}$$

- We will call a solution to the Cauchy problem for the Fokker–Planck equation (2) a **classical solution** if:

  i) $u \in C^{2,1}(\mathbb{R}^d, \mathbb{R}^+)$.

  ii) $\forall T > 0$ there exists a $c > 0$ such that

  $$\|u(t,x)\|_{L^\infty(0,T)} \leqslant c e^{\alpha \|x\|^2}$$

  iii) $\lim_{t \to 0} u(t,x) = f(x)$.

Theorem 1. *Assume that conditions* (3) *and* (4) *are satisfied, and assume that* $|f| \leqslant ce^{\alpha\|x\|^2}$. *Then there exists a unique classical solution to the Cauchy problem for the Fokker–Planck equation. Furthermore, there exist positive constants* K, δ *so that*

$$|p|,\ |p_t|,\ \|\nabla p\|,\ \|D^2 p\| \leqslant K t^{(-n+2)/2} \exp\left(-\frac{1}{2t}\delta\|x\|^2\right).$$

- This estimate enables us to multiply the Fokker-Planck equation by monomials x^n and then to integrate over $\mathbb{R}^d$ and to integrate by parts.

The FP equation as a conservation law

- We can define the **probability current** to be the vector whose ith component is

$$J_i := a_i(x)p - \frac{1}{2}\sum_{j=1}^{d} \frac{\partial}{\partial x_j}\big(b_{ij}(x)p\big).$$

- The Fokker–Planck equation can be written as a **continuity equation**:

$$\frac{\partial p}{\partial t} + \nabla \cdot J = 0.$$

- Integrating the FP equation over $\mathbb{R}^d$ and integrating by parts on the right hand side of the equation we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^d} p(x,t)\,dx = 0.$$

- Consequently:

$$\|p(\cdot,t)\|_{L^1(\mathbb{R}^d)} = \|p(\cdot,0)\|_{L^1(\mathbb{R}^d)} = 1.$$

- Set $a(t,x) \equiv 0$, $b(t,x) \equiv 2D > 0$. The Fokker-Planck equation becomes:

$$\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}, \quad p(x,s|y,s) = \delta(x-y).$$

- This is the heat equation, which is the Fokker-Planck equation for Brownian motion (Einstein, 1905). Its solution is

$$p_W(x,t|y,s) = \frac{1}{\sqrt{2\pi D(t-s)}} \exp\left(-\frac{(x-s)^2}{2D(t-s)} \right).$$

- Assume that the initial distribution is

$$p_W(x,s|y,s) = W(y,s).$$

- The solution of the Fokker-Planck equation for Brownian motion with this initial distribution is

$$P_W(x,t) = \int p(x,t|y,s)W(y,s)\,dy.$$

- The Gaussian distribution is the **fundamental solution** (Green's function) of the heat equation (i.e. the Fokker-Planck equation for Brownian motion).

- Set $a(t,x) = -\alpha x$, $b(t,x) \equiv 2D > 0$:

$$\frac{\partial p}{\partial t} = \alpha \frac{\partial (xp)}{\partial x} + D \frac{\partial^2 p}{\partial x^2}.$$

- This is the Fokker-Planck equation for the Ornstein-Uhlenbeck process (Ornstein-Uhlenbeck, 1930). Its solution is

$$p_{OU}(x,t|y,s) = \sqrt{\frac{\alpha}{2\pi D(1 - e^{-2\alpha(t-s)})}} \exp\left(-\frac{\alpha(x - e^{-\alpha(t-s)}y)^2}{2D(1 - e^{-2\alpha(t-s)})} \right).$$

- Proof: take the Fourier transform in x, use the method of characteristics and take the inverse Fourier transform.

- Set $y = 0$, $s = 0$. Notice that

$$\lim_{\alpha \to 0} p_{OU}(x,t) = p_W(x,t).$$

- Thus, in the limit where the friction coefficient goes to 0, we recover distribution function of BM from the DF of the OU processes.

- Notice also that

$$\lim_{t \to +\infty} p_{OU}(x,t) = \sqrt{\frac{\alpha}{2\pi D}} \exp\left(-\frac{\alpha x^2}{2D}\right).$$

- Thus, the Ornstein-Uhlenbeck process is an ergodic Markov process. Its invariant measure is Gaussian.

- We can calculate all moments of the OU process.

- Define the nth moment of the OU process:

$$M_n = \int_{\mathbb{R}} x^n p(x,t)\,dx, \quad n = 0, 1, 2, \ldots.$$

- Let $n = 0$. We integrate the FP equation over $\mathbb{R}$ to obtain:

$$\int \frac{\partial p}{\partial t} = \alpha \int \frac{\partial (xp)}{\partial x} + D \int \frac{\partial^2 p}{\partial x^2} = 0,$$

- after an integration by parts and using the fact that $p(x,t)$ decays sufficiently fast at infinity. Consequently:

$$\frac{d}{dt} M_0 = 0 \quad \Rightarrow \; M_0(t) = M_0(0) = 1.$$

- In other words:

$$\frac{d}{dt} \|p\|_{L^1(\mathbb{R})} = 0 \quad \Rightarrow \; p(x,t) = p(x, t = 0).$$

- Consequently: **probability is conserved**.

- Let $n = 1$. We multiply the FP equation for the OU process by x, integrate over $\mathbb{R}$ and perform and integration by parts to obtain:
$$\frac{d}{dt} M_1 = -\alpha M_1.$$
- Consequently, the first moment converges **exponentially fast** to 0:
$$M_1(t) = e^{-\alpha t} M_1(0).$$

- Let now $n \geqslant 2$. We multiply the FP equation for the OU process by x^n and integrate by parts (once on the first term on the RHS and twice on the second) to obtain:

$$\frac{d}{dt}\int x^n p = -\alpha n \int x^n p + Dn(n-1)\int x^{n-2} p.$$

- Or, equivalently:

$$\frac{d}{dt} M_n = -\alpha n M_n + Dn(n-1) M_{n-2}, \quad n \geqslant 2.$$

- This is a first order linear inhomogeneous differential equation. We can solve it using the variation of constants formula:

$$M_n(t) = e^{-\alpha n t} M_n(0) + Dn(n-1)\int_0^t e^{-\alpha n (t-s)} M_{n-2}(s)\, ds.$$

- The stationary moments of the OU process are:

$$
\begin{aligned}
\langle x^n \rangle_{OU} &= \sqrt{\frac{\alpha}{2\pi D}} \int_{\mathbb{R}} x^n e^{-\frac{\alpha x^2}{2D}}\, dx \\
&= \begin{cases} 1.3\ldots(n-1)\left(\frac{D}{\alpha}\right)^{n/2}, & n \,\text{even}, \\ 0, & n \,\text{odd}. \end{cases}
\end{aligned}
$$

- We have that

$$\lim_{t \to \infty} M_n(t) = \langle x^n \rangle_{OU}.$$

- If the initial conditions of the OU process are stationary, then:

$$M_n(t) = M_n(0) = \langle x^n \rangle_{OU}.$$

- set $a(x) = \mu x, \;\; b(x) = \frac{1}{2}\sigma x^2$. This is the **geometric Brownian motion**. The generator of this process is

$$\mathcal{L} = \mu x \frac{\partial}{\partial x} + \frac{\sigma^2 x^2}{2} \frac{\partial^2}{\partial x^2}.$$

- Notice that this operator is not uniformly elliptic.
- The Fokker-Planck equation of the geometric Brownian motion is:

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left(\mu x\right) + \frac{\partial^2}{\partial x^2}\left(\frac{\sigma^2 x^2}{2} p\right).$$

- We can easily obtain an equation for the nth moment of the geometric Brownian motion:

$$\frac{d}{dt}M_n = \Big(\mu n + \frac{\sigma^2}{2}n(n-1)\Big)M_n, \quad n \geqslant 2.$$

- The solution of this equation is

$$M_n(t) = e^{(\mu+(n-1)\frac{\sigma^2}{2})nt}M_n(0), \quad n \geqslant 2$$

- and

$$M_1(t) = e^{\mu t}M_1(0).$$

- Notice that the nth moment might diverge as $t \to \infty$, depending on the values of μ and σ:

$$\lim_{t\to\infty} M_n(t) = \begin{cases} 0, & \frac{\sigma^2}{2} < -\frac{\mu}{n-1}, \\ M_n(0), & \frac{\sigma^2}{2} = -\frac{\mu}{n-1}, \\ +\infty, & \frac{\sigma^2}{2} > -\frac{\mu}{n-1}. \end{cases}$$

- Let $V(x) = \frac{1}{2}\alpha x^2$. The generator of the OU process can be written as:

$$\mathcal{L} = -\partial_x V \partial_x + D\partial_x^2.$$

- Consider diffusion processes with a potential $V(x)$, not necessarily quadratic:

$$\mathcal{L} = -\nabla V(x) \cdot \nabla + D\Delta. \tag{5}$$

- This is a **gradient flow** perturbed by noise whose strength is $D = k_B T$ where k_B is Boltzmann's constant and T the absolute temperature.

- The corresponding stochastic differential equation is

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2D}\,dW_t.$$

- The corresponding FP equation is:

$$\frac{\partial p}{\partial t} = \nabla \cdot (\nabla V p) + D \Delta p. \tag{6}$$

- It is not possible to calculate the time dependent solution of this equation for an arbitrary potential. We can, however, alwas calculate the stationary solution.

Proposition 1. *Assume that $V(x)$ is smooth and that*

$$e^{-V(x)/D} \in L^1(\mathbb{R}^d). \tag{7}$$

Then the Markov process with generator (5) *is ergodic. The unique invariant distribution is the* **Gibbs distribution**

$$p(x) = \frac{1}{Z} e^{-V(x)/D} \tag{8}$$

where the normalization factor Z is the **partition function**

$$Z = \int_{\mathbb{R}^d} e^{-V(x)/D}\, dx.$$

- The fact that the Gibbs distribution is an invariant distribution follows by direct substitution. Uniqueness follows from a PDEs argument (see discussion below).
- It is more convenient to "normalize" the solution of the Fokker-Planck equation wrt the invariant distribution.

Proposition 2. *Let $p(x,t)$ be the solution of the Fokker-Planck equation* (6)*, assume that* (7) *holds and let $\rho(x)$ be the Gibbs distribution* (8)*. Define $h(x,t)$ through*

$$p(x,t) = h(x,t)\rho(x).$$

Then the function h satisfies the **backward Kolmogorov equation***:*

$$\frac{\partial h}{\partial t} = -\nabla V \cdot \nabla h + D\Delta h, \quad h(x,0) = p(x,0)\rho^{-1}(x). \tag{9}$$

Proof. The initial condition follows from the definition of h. We calculate the gradient and Laplacian of p:

$$\nabla p = \rho \nabla h - \rho h D^{-1} \nabla V$$

and

$$\Delta p = \rho \Delta h - 2\rho D^{-1} \nabla V \cdot \nabla h + h D^{-1} \Delta V \rho + h |\nabla V|^2 D^{-2} \rho.$$

We substitute these formulas into the FP equation to obtain

$$\rho \frac{\partial h}{\partial t} \quad = \quad \rho \Big(- \nabla V \cdot \nabla h + D \Delta h \Big),$$

from which the claim follows. $\square$

- Consequently, in order to study properties of solutions to the FP equation, it is sufficient to study the backward equation (9).
- The generator $\mathcal{L}$ is self-adjoint, in the right function space.
- We define the weighted L^2 space L^2_ρ:

$$L^2_\rho = \Big\{ f \Big| \int_{\mathbb{R}^d} |f|^2 \rho(x)\, dx < \infty \Big\},$$

- where $\rho(x)$ is the Gibbs distribution. This is a Hilbert space with inner product

$$(f, h)_\rho = \int_{\mathbb{R}^d} f h \rho(x)\, dx.$$

Proposition 3. *Assume that $V(x)$ is a smooth potential and assume that condition (7) holds. Then the operator*

$$\mathcal{L} = -\nabla V(x) \cdot \nabla + D\Delta$$

is self-adjoint in L^2_ρ. Furthermore, it is non-positive, its kernel consists of constants.

Proof. Let $f, \in C_0^2(\mathbb{R}^d)$. We calculate

$$\begin{aligned}
(\mathcal{L}f, h)_\rho &= \int_{\mathbb{R}^d} (-\nabla V \cdot \nabla + D\Delta) f h \rho \, dx \\
&= \int_{\mathbb{R}^d} (\nabla V \cdot \nabla f) h \rho \, dx - D \int_{\mathbb{R}^d} \nabla f \nabla h \rho \, dx - D \int_{\mathbb{R}^d} \nabla f h \nabla \rho \, dx \\
&= -D \int_{\mathbb{R}^d} \nabla f \cdot \nabla h \rho \, dx,
\end{aligned}$$

from which self-adjointness follows.

If we set $f = h$ in the above equation we get

$$(\mathcal{L}f, f)_\rho = -D\|\nabla f\|_\rho^2,$$

which shows that $\mathcal{L}$ is non-positive.

Clearly, constants are in the null space of $\mathcal{L}$. Assume that $f \in \mathcal{N}(\mathcal{L})$. Then, from the above equation we get

$$0 = -D\|\nabla f\|_\rho^2,$$

and, consequently, f is a constant. $\square$

Remark 1. *The expression* $(-\mathcal{L}f, f)_\rho$ *is called the* **Dirichlet form** *of the operator* $\mathcal{L}$. *In the case of a gradient flow, it takes the form*

$$(-\mathcal{L}f, f)_\rho = D\|\nabla f\|_\rho^2. \tag{10}$$

- Using the properties of the generator $\mathcal{L}$ we can show that the solution of the Fokker-Planck equation converges to the Gibbs distribution exponentially fast.
- For this we need the following result.

Proposition 4. *Assume that the potential V satisfies the convexity condition*

$$D^2 V \geqslant \lambda I.$$

Then the corresponding Gibbs measure satisfies the Poincaré inequality with constant λ:

$$\int_{\mathbb{R}^d} f\rho = 0 \quad \Rightarrow \quad \|\nabla f\|_\rho \geqslant \sqrt{\lambda}\|f\|_\rho. \tag{11}$$

Theorem 2. *Assume that $p(x,0) \in L^2(e^{V/D})$. Then the solution $p(x,t)$ of the Fokker-Planck equation* (6) *converges to the Gibbs distribution exponentially fast:*

$$\|p(\cdot,t) - Z^{-1}e^{-V}\|_{\rho^{-1}} \leqslant e^{-\lambda D t}\|p(\cdot,0) - Z^{-1}e^{-V}\|_{\rho^{-1}}. \tag{12}$$

Proof. We Use (9), (10) and (11) to calculate

$$\begin{aligned} -\frac{d}{dt}\|(h-1)\|_\rho^2 &= -2\left(\frac{\partial h}{\partial t}, h-1\right)_\rho = -2\left(\mathcal{L}h, h-1\right)_\rho \\ &= \left(-\mathcal{L}(h-1), h-1\right)_\rho = 2D\|\nabla(h-1)\|_\rho \\ &\geqslant 2D\lambda\|h-1\|_\rho^2. \end{aligned}$$

Our assumption on $p(\cdot,0)$ implies that $h(\cdot,0) \in L^2_\rho$. Consequently, the above calculation shows that

$$\|h(\cdot,t) - 1\|_\rho \leqslant e^{-\lambda D t}\|H(\cdot,0) - 1\|_\rho.$$

This, and the definition of h, $p = \rho h$, lead to (12). $\square$

- The assumption

$$\int_{\mathbb{R}^d} |p(x,0)|^2 Z^{-1} e^{V/D} < \infty$$

- is very restrictive (think of the case where $V = x^2$).
- The function space $L^(\rho^{-1}) = L^2(e^{-V/D})$ in which we prove convergence is not the right space to use. Since $p(\cdot, t) \in L^1$, ideally we would like to prove exponentially fast convergence in L^1.
- We can prove convergence in L^1 using the theory of **logarithmic Sobolev inequalities**. In fact, we can also prove convergence in **relative entropy**:

$$H(p|\rho_V) := \int_{\mathbb{R}^d} p \ln \left(\frac{p}{\rho_V} \right) \, dx.$$

- The relative entropy norm controls the L^1 norm:

$$\|\rho_1 - \rho_2\|_{L^1} \leqslant C H(\rho_1|\rho_2)$$

- Using a logarithmic Sobolev inequality, we can prove exponentially fast convergence to equilibrium, assuming only that the relative entropy of the initial conditions is finite.

Theorem 3. *Let p denote the solution of the Fokker–Planck equation* (6) *where the potential is smooth and uniformly convex. Assume that the the initial conditions satisfy*

$$H(p(\cdot,0)|\rho_V) < \infty.$$

Then p converges to the Gibbs distribution exponentially fast in relative entropy:

$$H(p(\cdot,t)|\rho_V) \leqslant e^{-\lambda D t} H(p(\cdot,0)|\rho_V).$$

- Convergence to equilibrium for **kinetic equations**, both linear and non-linear (e.g., the Boltzmann equation) has been studied extensively in the last decade.
- It has been recognized that the relative entropy plays a very important role.
- For more information see
- *On the trend to equilibrium for the Fokker-Planck equation: an interplay between physics and functional analysis* by P.A. Markowich and C. Villani, 1999.

- Consider the generator of a gradient stochastic flow with a uniformly convex potential

$$\mathcal{L} = -\nabla V \cdot \nabla + D\Delta. \tag{13}$$

- We know that

  i) $\mathcal{L}$ is a non-positive self-adjoint operator on L^2_ρ.

  ii) It has a spectral gap:

$$(\mathcal{L}f, f)_\rho \leqslant -D\lambda \|f\|_\rho^2$$

  where λ is the Poincaré constant of the potential V.

- The above imply that we can study the spectral problem for $-\mathcal{L}$:

$$-\mathcal{L}f_n = \lambda_n f_n, \quad n = 0, 1, \dots$$

Eigenfunction Expansions

- The operator $-\mathcal{L}$ has real, discrete spectrum with

$$0 = \lambda_0 < \lambda_1 < \lambda_2 < \dots$$

- Furthermore, the eigenfunctions $\{f_j\}_{j=1}^{infty}$ form an orthonormal basis in L^2_ρ: we can express every element of L^2_ρ in the form of a generalized Fourier series:

$$\phi = \sum_{n=0}^{\infty} \phi_n f_n, \quad \phi_n = (\phi, f_n)_\rho \tag{14}$$

- with $(f_n, f_m)_\rho = \delta_{nm}$.
- This enables us to solve the time dependent Fokker–Planck equation in terms of an eigenfunction expansion.
- Consider the backward Kolmogorov equation (9).
- We assume that the initial conditions $h_0(x) = \phi(x) \in L^2_\rho$ and consequently we can expand it in the form (14).

- We look for a solution of (9) in the form

$$h(x,t) = \sum_{n=0}^{\infty} h_n(t) f_n(x).$$

- We substitute this expansion into the backward Kolmogorov equation:

$$\begin{aligned} \frac{\partial h}{\partial t} &= \sum_{n=0}^{\infty} \dot{h}_n f_n = \mathcal{L}\left(\sum_{n=0}^{\infty} h_n f_n\right) && (15) \\ &= \sum_{n=0}^{\infty} -\lambda_n h_n f_n. && (16) \end{aligned}$$

- We multiply this equation by f_m, integrate wrt the Gibbs measure and use the orthonormality of the eigenfunctions to obtain the sequence of equations

$$\dot{h}_n = -\lambda_n h_n, \quad n = 0, 1,$$

- The solution is

$$h_0(t) = \phi_0, \quad h_n(t) = e^{-\lambda_n t}\phi_n, \; n = 1, 2, \dots$$

- Notice that

$$\begin{aligned} 1 &= \int_{\mathbb{R}^d} p(x,0)\,dx = \int_{\mathbb{R}^d} p(x,t)\,dx \\ &= \int_{\mathbb{R}^d} h(x,t) Z^{-1} e^{\beta V}\,dx = (h,1)_\rho = (\phi,1)_\rho \\ &= \phi_0. \end{aligned}$$

- Consequently, the solution of the backward Kolmogorov equation is

$$h(x,t) = 1 + \sum_{n=1}^{\infty} e^{-\lambda_n t} \phi_n f_n.$$

- This expansion, together with the fact that all eigenvalues are positive ($n \geqslant 1$), shows that the solution of the backward Kolmogorov equation converges to 1 exponentially fast.

- The solution of the Fokker–Planck equation is

$$p(x,t) = Z^{-1} e^{-\beta V(x)} \left(1 + \sum_{n=1}^{\infty} e^{-\lambda_n t} \phi_n f_n \right).$$

- The Fokker–Planck operator of a general diffusion process is not self-adjoint in general.
- In fact, it is self-adjoint **if and only if** the drift term is the gradient of a potential (Nelson, ≈ 1960). This is also true in infinite dimensions (Stochastic PDEs).
- Markov Processes whose generator is a self-adjoint operator are called **reversible**: for all $t \in [0, T]$ X_t and X_{T-t} have the same transition probability (when X_t is statinary).
- Reversibility is equivalent to the invariant measure being a Gibbs measure.
- See *Thermodynamics of the general duffusion process: time-reversibility and entropy production*, H. Qian, M. Qian, X. Tang, J. Stat. Phys., 107, (5/6), 2002, pp. 1129–1141.

- We can study the Fokker-Planck equation for a gradient flow by mapping it to a Schrödinger equation.

Proposition 5. *The Fokker–Planck operator for a gradient flow can be written in the self-adjoint form*

$$\frac{\partial p}{\partial t} = D\nabla \cdot \left(e^{-V/D}\nabla \left(e^{V/D}p\right)\right). \tag{17}$$

Define now $\psi(x,t) = e^{V/2D}p(x,t)$. Then ψ solves the PDE

$$\frac{\partial \psi}{\partial t} = D\Delta\psi - U(x)\psi, \quad U(x) := \frac{|\nabla V|^2}{4D} - \frac{\Delta V}{2}. \tag{18}$$

Let $\mathcal{H} := -D\Delta + U$. Then $\mathcal{L}^*$ and $\mathcal{H}$ have the same eigenvalues. The nth eigenfunction ϕ_n of $\mathcal{L}^*$ and the nth eigenfunction ψ_n of $\mathcal{H}$ are associated through the transformation

$$\psi_n(x) = \phi_n(x)\exp\left(\frac{V(x)}{2D}\right).$$

Remarks

i) From equation (17) shows that the FP operator can be written in the form

$$\mathcal{L}^* \cdot = D\nabla \cdot \left(e^{-V/D} \nabla \left(e^{V/D} \cdot \right) \right).$$

ii) The operator that appears on the right hand side of eqn. (18) has the form of a **Schrödinger operator**:

$$-\mathcal{H} = -D\Delta + U(x).$$

iii) The spectral problem for the FP operator can be transformed into the spectral problem for a Schrödinger operator. We can thus use all the available results from quantum mechanics to study the FP equation and the associated SDE.

iv) In particular, the weak noise asymptotics $D \ll 1$ is equivalent to the semiclassical approximation from quantum mechanics.

Proof of Prop. 5. We calculate

$$\begin{aligned} D\nabla \cdot \left(e^{-V/D}\nabla\left(e^{V/D}f\right)\right) &= D\nabla\cdot\left(e^{-V/D}\left(D^{-1}\nabla V f + \nabla f\right)e^{V/D}\right) \\ &= \nabla\cdot\left(\nabla V f + D\nabla f\right) = \mathcal{L}^* f. \end{aligned}$$

Consider now the eigenvalue problem for the FP operator:

$$-\mathcal{L}^*\phi_n = \lambda_n \phi_n.$$

Set $\phi_n = \psi_n \exp\left(-\frac{1}{2D}V\right)$. We calculate $-\mathcal{L}^*\phi_n$:

$$\begin{aligned} -\mathcal{L}^*\phi_n &= -D\nabla\cdot\left(e^{-V/D}\nabla\left(e^{V/D}\psi_n e^{-V/2D}\right)\right) \\ &= -D\nabla\cdot\left(e^{-V/D}\left(\nabla\psi_n + \frac{\nabla V}{2D}\psi_n\right)e^{V/2D}\right) \\ &= \left(-D\Delta\psi_n + \left(-\frac{|\nabla V|^2}{4D} + \frac{\Delta V}{2D}\right)\psi_n\right)e^{-V/2D} = e^{-V/2D}\mathcal{H}\psi_n. \end{aligned}$$

From this we conclude that $e^{-V/2D}\mathcal{H}\psi_n = \lambda_n\psi_n e^{-V/2D}$ from which the equivalence between the two eigenvalue problems follows. $\square$

Remarks

i) We can rewrite the Schrödinger operator in the form

$$\mathcal{H} = D\mathcal{A}^*\mathcal{A}, \quad \mathcal{A} = \nabla + \frac{\nabla U}{2D}, \quad \mathcal{A}^* = -\nabla + \frac{\nabla U}{2D}.$$

ii) These are **creation** and **annihilation** operators. They can also be written in the form

$$\mathcal{A}\cdot = e^{-U/2D}\nabla\left(e^{U/2D}\cdot\right), \quad \mathcal{A}^*\cdot = e^{U/2D}\nabla\left(e^{-U/2D}\cdot\right)$$

iii) The forward the backward Kolmogorov operators have the same eigenvalues. Their eigenfunctions are related through

$$\phi_n^B = \phi_n^F \exp\left(-V/D\right),$$

where ϕ_n^B and ϕ_n^F denote the eigenfunctions of the backward and forward operators, respectively.

- The generator of the OU process is

$$\mathcal{L} = -y\frac{d}{dy} + D\frac{d^2}{dy^2} \tag{19}$$

- The OU process is an ergodic Markov process whose unique invariant measure is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$ with density $\rho(y) \in C^\infty(\mathbb{R})$

$$\rho(y) = \frac{1}{\sqrt{2\pi D}} e^{-\frac{y^2}{2D}}.$$

- Let L^2_ρ denote the closure of C^∞ functions with respect to the norm

$$\|f\|^2_\rho = \int_{\mathbb{R}} f(y)^2 \rho(y)\, dy.$$

- The space L^2_ρ is a Hilbert space with inner product

$$(f, g)_\rho = \int_{\mathbb{R}} f(y) g(y) \rho(y)\, dy.$$

The Ornstein–Uhlenbeck Process and Hermite Polynomials

- Consider the eigenvalue problem for $\mathcal{L}$:

$$-\mathcal{L} f_n = \lambda_n f_n.$$

- The operator $\mathcal{L}$ has discrete spectrum in L^2_ρ:

$$\lambda_n = n, \quad n \in \mathcal{N}.$$

- The corresponding eigenfunctions are the normalized Hermite polynomials:

$$f_n(y) = \frac{1}{\sqrt{n!}} H_n\left(\frac{y}{\sqrt{D}}\right), \tag{20}$$

where

$$H_n(y) = (-1)^n e^{\frac{y^2}{2}} \frac{d^n}{dy^n}\left(e^{-\frac{y^2}{2}}\right).$$

- The first few Hermite polynomials are:

$$\begin{aligned} H_0(y) &= 1, \\ H_1(y) &= y, \\ H_2(y) &= y^2 - 1, \\ H_3(y) &= y^3 - 3y, \\ H_4(y) &= y^4 - 3y^2 + 3, \\ H_5(y) &= y^5 - 10y^3 + 15y. \end{aligned}$$

- H_n is a polynomial of degree n.
- Only odd (even) powers appear in H_n when n is odd (even).

Lemma 1. *The eigenfunctions $\{f_n(y)\}_{n=1}^{\infty}$ of the generator of the OU process $\mathcal{L}$ satisfy the following properties.*

i) They form an orthonormal set in L^2_ρ:

$$(f_n, f_m)_\rho = \delta_{nm}.$$

ii) $\{f_n(y) : n \in \mathcal{N}\}$ is an orthonormal basis in L^2_ρ.

iii) Define the creation and annihilation operators on $C^1(\mathbb{R})$ by

$$A_+\phi(y) = \frac{1}{\sqrt{D(n+1)}}\left(-D\frac{d\phi}{dy}(y) + y\phi(y)\right), \quad y \in \mathbb{R}$$

and

$$A_-\phi(y) = \sqrt{\frac{D}{n}}\frac{d\phi}{dy}(y).$$

Then

$$A_+ f_n = f_{n+1} \quad \text{and} \quad A_- f_n = f_{n-1}. \tag{21}$$

iv) The eigenfunctions f_n satisfy the following recurrence relation

$$y f_n(y) = \sqrt{Dn} f_{n-1}(y) + \sqrt{D(n+1)} f_{n+1}(y), \quad n \geqslant 1. \tag{22}$$

v) The function

$$H(y; \lambda) = e^{\lambda y - \frac{\lambda^2}{2}}$$

is a generating function for the Hermite polynomials. In particular

$$H\left(\frac{y}{\sqrt{D}}; \lambda\right) = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} f_n(y), \quad \lambda \in \mathbb{C}, \, y \in \mathbb{R}.$$

- Consider a diffusion process in two dimensions for the variables q (position) and momentum p. The generator of this Markov process is

$$\mathcal{L} = p \cdot \nabla_q - \nabla_q V \nabla_p + \gamma(-p\nabla_p + D\Delta_p). \tag{23}$$

- The $L^2(dpdq)$-adjoint is

$$\mathcal{L}^* \rho = -p \cdot \nabla_q \rho - \nabla_q V \cdot \nabla_p \rho + \gamma \left(\nabla_p (p\rho) + D\Delta_p \rho \right).$$

- The corresponding FP equation is:

$$\frac{\partial p}{\partial t} = \mathcal{L}^* p.$$

- The corresponding stochastic differential equations is the **Langevin equation**

$$\ddot{X}_t = -\nabla V(X_t) - \gamma \dot{X}_t + \sqrt{2\gamma D}\dot{W}_t. \tag{24}$$

- This is Newton's equation perturbed by dissipation and noise.

- The Klein-Kramers-Chandrasekhar equation was first derived by Kramers in 1923 and was studied by Kramers in his famous paper "Brownian motion in a field of force and the diffusion model of chemical reactions", Physica 7(1940), pp. 284-304.
- Notice that $\mathcal{L}^*$ is not a uniformly elliptic operator: there are second order derivatives only with respect to p and not q. This is an example of a degenerate elliptic operator. It is, however, **hypoelliptic**: we can still prove existence and uniqueness of solutions for the FP equation, and obtain estimates on the solution.
- It is not possible to obtain the solution of the FP equation for an arbitrary potential.
- We can calculate the (unique normalized) solution of the stationary Fokker-Planck equation.

Proposition 6. *Assume that $V(x)$ is smooth and that*

$$e^{-V(x)/D} \in L^1(\mathbb{R}^d).$$

Then the Markov process with generator (23) is ergodic. The unique invariant distribution is the **Maxwell-Boltzmann distribution**

$$\rho(p, q) = \frac{1}{Z} e^{-\beta H(p,q)} \tag{25}$$

where

$$H(p, q) = \frac{1}{2}\|p\|^2 + V(q)$$

is the **Hamiltonian**, $\beta = (k_B T)^{-1}$ *is the* **inverse temperature** *and the normalization factor Z is the* **partition function**

$$Z = \int_{\mathbb{R}^{2d}} e^{-\beta H(p,q)}\, dpdq.$$

- It is possible to obtain rates of convergence in either a weighted L^2-norm or the relative entropy norm.

$$H(p(\cdot,t)|\rho) \leqslant Ce^{-\alpha t}.$$

- The proof of this result is very complicated, since the generator $\mathcal{L}$ is degenerate and non-selfadjoint.

- See F. Herau and F. Nier, *Isotropic hypoellipticity and trend to equilibrium for the Fokker-Planck equation with a high-degree potential*, Arch. Ration. Mech. Anal., 171(2),(2004), 151–218.

- The phase-space Fokker-Planck equation can be written in the form
$$\frac{\partial \rho}{\partial t} + p \cdot \nabla_q \rho - \nabla_q V \cdot \nabla_p \rho = Q(\rho, f_B)$$
- where the *collision operator* has the form
$$Q(\rho, f_B) = D \nabla \cdot \left(f_B \nabla \left(f_B^{-1} \rho \right) \right).$$
- The Fokker-Planck equation has a similar structure to the Boltzmann equation (the basic equation in the kinetic theory of gases), with the difference that the collision operator for the FP equation is linear.
- Convergence of solutions of the Boltzmann equation to the Maxwell-Boltzmann distribution has also been proved. See
- L. Desvillettes and C. Villani: On the trend to global equilibrium for spatially inhomogeneous kinetic systems: the Boltzmann equation. Invent. Math. 159, 2 (2005), 245-316.

- We can study the backward and forward Kolmogorov equations for (24) by expanding the solution with respect to the Hermite basis.

- We consider the problem in 1d. We set $D = 1$. The generator of the process is:

$$\begin{aligned} \mathcal{L} &= p\partial_q - V'(q)\partial_p + \gamma\left(-p\partial_p + \partial_p^2\right). \\ &=: \mathcal{L}_1 + \gamma\mathcal{L}_0, \end{aligned}$$

- where

$$\mathcal{L}_0 := -p\partial_p + \partial_p^2 \quad \text{and} \quad \mathcal{L}_1 := p\partial_q - V'(q)\partial_p.$$

- The backward Kolmogorov equation is

$$\frac{\partial h}{\partial t} = \mathcal{L}h. \tag{26}$$

- The solution should be an element of the weighted L^2-space

$$L^2_\rho = \left\{ f | \int_{\mathbb{R}^2} |f|^2 Z^{-1} e^{-\beta H(p,q)}\, dpdq < \infty \right\}.$$

- We notice that the invariant measure of our Markov process is a product measure:

$$e^{-\beta H(p,q)} = e^{-\beta \frac{1}{2}|p|^2} e^{-\beta V(q)}.$$

- The space $L^2(e^{-\beta \frac{1}{2}|p|^2}\, dp)$ is spanned by the Hermite polynomials. Consequently, we can expand the solution of (26) into the basis of Hermite basis:

$$h(p,q,t) = \sum_{n=0}^{\infty} h_n(q,t) f_n(p), \tag{27}$$

- where $f_n(p) = 1/\sqrt{n!} H_n(p)$.

- Our plan is to substitute (27) into (26) and obtain a sequence of equations for the coefficients $h_n(q,t)$.
- We have:

$$\mathcal{L}_0 h = \mathcal{L}_0 \sum_{n=0}^{\infty} h_n f_n = -\sum_{n=0}^{\infty} n h_n f_n$$

- Furthermore

$$\mathcal{L}_1 h = -\partial_q V \partial_p h + p \partial_q h.$$

- We calculate each term on the right hand side of the above equation separately. For this we will need the formulas

$$\partial_p f_n = \sqrt{n} f_{n-1} \quad \text{and } p f_n = \sqrt{n} f_{n-1} + \sqrt{n+1} f_{n+1}.$$

$$
\begin{aligned}
p\partial_q h &= p\partial_q \sum_{n=0}^{\infty} h_n f_n = p\partial_p h_0 + \sum_{n=1}^{\infty} \partial_q h_n p f_n \\
&= \partial_q h_0 f_1 + \sum_{n=1}^{\infty} \partial_q h_n \left(\sqrt{n} f_{n-1} + \sqrt{n+1} f_{n+1}\right) \\
&= \sum_{n=0}^{\infty} (\sqrt{n+1}\partial_q h_{n+1} + \sqrt{n}\partial_q h_{n-1}) f_n
\end{aligned}
$$

- with $h_{-1} \equiv 0$.
- Furthermore

$$
\begin{aligned}
\partial_q V \partial_p h &= \sum_{n=0}^{\infty} \partial_q V h_n \partial_p f_n = \sum_{n=0}^{\infty} \partial_q V h_n \sqrt{n} f_{n-1} \\
&= \sum_{n=0}^{\infty} \partial_q V h_{n+1} \sqrt{n+1} f_n .
\end{aligned}
$$

- Consequently:

$$\begin{aligned} \mathcal{L}h &= \mathcal{L}_1 + \gamma \mathcal{L}_1 h \\ &= \sum_{n=0}^{\infty} \big(-\gamma n h_n + \sqrt{n+1}\partial_q h_{n+1} \\ &\quad + \sqrt{n}\partial_q h_{n-1} + \sqrt{n+1}\partial_q V h_{n+1} \big) f_n \end{aligned}$$

- Using the orthonormality of the eigenfunctions of $\mathcal{L}_0$ we obtain the following set of equations which determine $\{h_n(q,t)\}_{n=0}^{\infty}$.

$$\begin{aligned} \dot{h}_n &= -\gamma n h_n + \sqrt{n+1}\partial_q h_{n+1} \\ &\quad + \sqrt{n}\partial_q h_{n-1} + \sqrt{n+1}\partial_q V h_{n+1}, \quad n = 0, 1, \ldots \end{aligned}$$

- This is set of equations is usually called the **Brinkman hierarchy** (1956).

- We can use this approach to develop a numerical method for solving the Klein-Kramers equation.
- For this we need to expand each coefficient h_n in an appropriate basis with respect to q.
- Obvious choices are other the Hermite basis (polynomial potentials) or the standard Fourier basis (periodic potentials).
- We will do this for the case of periodic potentials.
- The resulting method is usually called the **continued fraction expansion**. See Risken (1989).

The Klein-Kramers-Chandrasekhar Equation

- The Hermite expansion of the distribution function wrt to the velocity is used in the study of various kinetic equations (including the Boltzmann equation). It was initiated by Grad in the late 40's.
- It quite often used in the approximate calculation of transport coefficients (e.g. diffusion coefficient).
- This expansion can be justified rigorously for the Fokker-Planck equation. See
- J. Meyer and J. Schröter, *Comments on the Grad Procedure for the Fokker-Planck Equation*, J. Stat. Phys. 32(1) pp.53-69 (1983).

Boundary conditions for the Fokker–Planck equation

- So far we have been studying the FP equation on $\mathbb{R}^d$.
- The boundary condition was that the solution decays sufficiently fast at infinity.
- For ergodic diffusion processes this is equivalent to requiring that the solution of the backward Kolmogorov equation is an element of $L^2(\mu)$ where μ is the invariant measure of the process.
- We can also study the FP equation in a bounded domain with appropriate boundary conditions.
- We can have **absorbing, reflecting** or **periodic boundary** conditions.

- Consider the FP equation posed in $\Omega \subset \mathbb{R}^d$ where Ω is a bounded domain with smooth boundary.
- Let $\mathbf{J}$ denote the probability current and let $\mathbf{n}$ be the unit normal vector to the surface.

  i) We specify reflecting boundary conditions by setting

$$\mathbf{n} \cdot \mathbf{J}(x, t) = 0, \quad on\ \partial\Omega.$$

  ii) We specify absorbing boundary conditions by setting

$$p(x, t) = 0, \quad on\ \partial\Omega.$$

iii) When the coefficient of the FP equation are periodic functions, we might also want to consider periodic boundary conditions, i.e. the solution of the FP equation is periodic in x with period equal to that of the coefficients.

- Reflecting BC correspond to the case where a particle which evolves according to the SDE corresponding to the FP equation gets reflected at the boundary.
- Absorbing BC correspond to the case where a particle which evolves according to the SDE corresponding to the FP equation gets absorbed at the boundary.
- There is a complete classification of boundary conditions in one dimension, the **Feller classification**: the BC can be **regular, exit, entrance** and **natural**.

REFERENCES

- A lot of information about methods for solving the Fokker-Planck equation can be found in Risken **The Fokker-Planck equation**, Springer, Berlin 1989.
- See also Gardiner **Handbook of Stochastic Methods**, Horsthemke and Lefever **Noise Induced Transitions**.
- For a mathematically rigorous treatment see the books of Friedman, Arnold on SDES.