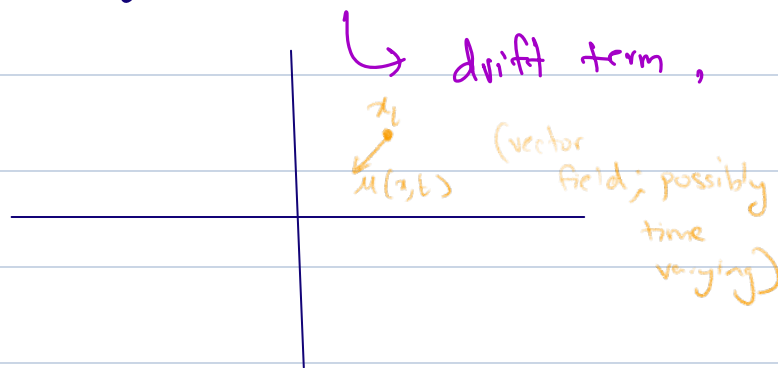


SDE Basics and the Fokker Planck Equation

References: 1. B. Oksendal, Stochastic Differential Equations, Springer, 2000
2. E. Ryu, Diffusion models, UCLA/SNU, 2024 (online slides).

ODE: $dx_t = \mu(x_t, t) dt$, $x_t \in \mathbb{R}^d$, x_0 given



Roughly: $x_{t+h} - x_t \approx \mu(x_t, t) \cdot h$
↳ small step.

SDE: $dx_t = \mu(x_t, t) dt + \sigma(x_t, t) dB_t$

random variable (pointing to dB_t)
↳ drift term (pointing to $\mu(x_t, t) dt$)
↳ diffusion term (pointing to $\sigma(x_t, t) dB_t$)
Brownian motion (pointing to dB_t)

$x_0 \sim p_0(\cdot)$ (IC sampled from a given dist. $p_0(\cdot)$),
 $t \in [0, T]$ (or $t \in [0, \infty)$)

B_t : Brownian motion
(i) $B_0 = 0$ a.s.
(ii) $(B_t - B_s) \sim N(0, t-s)$
(iii) Independent increments.

What does this mean?

1

$$(X_{t+h} - X_t) \approx \mu(X_t, t) ((t+h) - t) + \sigma(X_t, t) (B_{t+h} - B_t)$$

$$\text{i.e.} \quad X_{t+h} \approx X_t + \mu(X_t, t) \cdot h + \sigma(X_t, t) (B_{t+h} - B_t)$$

small drift

small Gaussian noise.

What does this imply? Let $f(\cdot)$ be a "nice" function whose derivatives exist, From Taylor's theorem,

$$f(x+a) = f(x) + f'(x)a + \frac{f''(x)a^2}{2} + \text{H.O.T.}$$

$$\therefore \text{For an ODE: } x_{t+h} \approx x_t + \mu(x_t, t)h$$

$$\begin{aligned} \therefore f(x_{t+h}) &\approx f(x_t) + f'(x_t) \cdot \mu(x_t, t)h + \\ &+ \frac{f''(x_t) \mu^2(x_t, t) h^2}{2} + \dots \end{aligned}$$

$\hookrightarrow O(h^2)$ small

$$\therefore \boxed{f(x_{t+h}) \approx f(x_t) + f'(x_t) \mu(x_t, t)h}$$

i.e., for a nice function $f(\cdot)$, a first-order

approximation suffices. Now, let us consider an SDE.

$$X_{t+h} \approx X_t + \underbrace{\mu(X_t, t) \cdot h}_{\text{drift}} + \underbrace{\sigma(X_t, t)(B_{t+h} - B_t)}_{\text{noise}}$$

$$\begin{aligned} \therefore F(X_{t+h}) &\approx F(X_t + \mu(X_t, t)h + \sigma(X_t, t)(B_{t+h} - B_t)) \\ &= F(X_t) + F'(X_t)\mu(X_t, t)h + F'(X_t)\sigma(X_t, t)(B_{t+h} - B_t) \\ &\quad + \underbrace{F''(X_t) \cdot \frac{\mu(X_t, t)^2 h^2}{2}}_{\text{red term}} + F''(X_t)\sigma^2(X_t, t)(B_{t+h} - B_t)^2 \\ &\quad + F''(X_t)\mu(X_t, t)h\sigma(X_t, t)(B_{t+h} - B_t) + \dots \end{aligned}$$

Now, two key facts: (1) $E[(B_{t+h} - B_t)] = 0$ mean ↓

$$(2) E[(B_{t+h} - B_t)^2] = h$$

↙
variance

Red term above can be ignored $\rightarrow O(h^2)$

Green term cannot be ignored because it scales as h in expectation

Blue term can be ignored because it is zero-mean
∴

$$f(x_{t+h}) \approx f(x_t) + f'(x_t) \mu(x_t, t) h + f'(x_t) \sigma(x_t, t) (B_{t+h} - B_t) + \frac{1}{2} f''(x_t) \sigma(x_t, t)^2 h$$

Takeaway: Second-order Taylor series expansion terms cannot be ignored for the stochastic setting.

Lipschitz continuity

Fact: Under "nice" conditions on $\mu(\cdot), \sigma(\cdot)$, $X_t, t \geq 0$ is well defined, has a unique t -continuous solution

Note: $dx_t = b(x_t)dt + \sigma(x_t)dB_t$ is intuitively Markovian, because to evolve $X_t \rightarrow X_{t+h}$, we only need to know X_t , and the evolution of B_t i.e., $B_t \rightarrow B_{t+h}$. Since B_t is indep increment, the past evolution of B_t does not affect its future.

Fact: Under nice conditions, $\{X_t, t \geq 0\}$ has the strong Markov property, i.e.,

$$E_x[F(X_{\tau+h}) | \mathcal{F}_\tau] = E_{x_\tau}[f(X_h)]$$

where τ is a stopping time.

② How does the pdf of X_t evolve?

$\{X_t, t \geq 0\}$ a Markov process.

$P_t(\cdot) \equiv$ pdf of X_t ; $X_0 \sim p_0(\cdot)$

↳ pdf at time t .

$\nearrow \in \mathbb{R}^d$.
d-dim "marginal" $\downarrow$ at time = 0.

Answer: The **Fokker-Planck Equation**
 $\equiv$ Kolmogorov Forward Equation
 $\equiv$ "Master" equation.

(See also wikipedia for the history of this equation)

The FP equations is a PDE that describes the time evolution of $P_t(\cdot)$. Below, we assume existence, unique of solution (holds under "usual, nice" conditions. (See [1]).

$$\frac{\partial}{\partial t} p_t(x) = - \sum_{i=1}^d \frac{\partial}{\partial x_i} (\mu_i(x, t) p_t(x))$$

$$+ \sum_{i=1}^d \sum_{j=1}^d \left(D_{ij}(x, t) \cdot \frac{\partial^2}{\partial x_i \partial x_j} p_t(x) \right)$$

where $D_{ij}(x, t) = \frac{1}{2} \sum_{r=1}^d \sigma_{ir}(x, t) \cdot \sigma_{jr}(x, t).$

Note: The Fokker-Planck Equation is closely related to the continuity equation for ODEs of density flow. If we set $\sigma = 0$ in the above equation, we get

$$\frac{\partial p}{\partial t} + \nabla \cdot (\mu p) = 0, \text{ where}$$

$$p \equiv p_t(x) \quad ; \quad \mu = \begin{pmatrix} \mu_1(x, t) \\ \vdots \\ \mu_d(x, t) \end{pmatrix}$$

and divergence: $\nabla = \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_d} \right)$

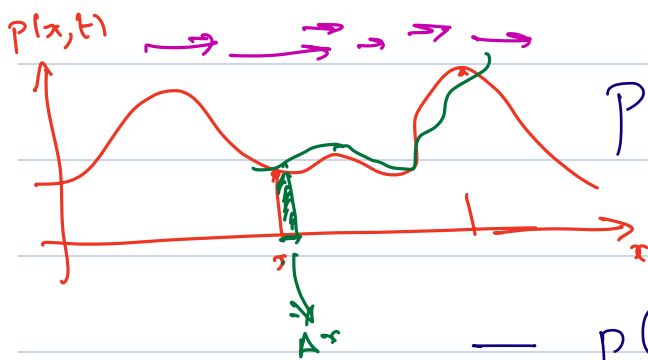
i.e., $\frac{\partial p}{\partial t} = - \sum_{i=1}^d \frac{\partial}{\partial x_i} (\mu_i(x, t) p_t(x)).$

Aside: Physics intuition on the continuity equation from conservation of mass

A rough sketch of the continuity equation.

$\mu \geq 0$ (assumption, for simplicity below)

$$p(x, t + \Delta t) \Delta x = p(x, t) \Delta x +$$



$$p(x - \Delta x, t) \cdot \Delta x - \frac{\mu(x - \Delta x, t) \cdot \Delta t}{\Delta x}$$

fraction of mass that moves displacement

bin size

$$- p(x, t) \Delta x \cdot \frac{\mu(x, t) \cdot \Delta t}{\Delta x}$$

$$\therefore \frac{p(x, t + \Delta t) - p(x, t)}{\Delta t} = \frac{p(x - \Delta x, t) \mu(x - \Delta x, t) - p(x, t) \mu(x, t)}{\Delta x}$$

i.e.,

$$\frac{\partial p}{\partial t} = - \frac{\partial (p \mu)}{\partial x}$$

If we start an ODE in a vector field $u(x, t)$, and with a random initial condition (IC), the density evolution is described by the continuity equation above.

This is also closely connected to the heat equation

$$\frac{\partial p}{\partial t} = \Delta p, \text{ i.e., } \frac{\partial p}{\partial t} = \sum_{i=1}^d \frac{\partial^2}{\partial x_i^2} p(t, x)$$

↳ Laplacian

Recall! $f = f(x_1, x_2, \dots, x_d)$ → Laplacian

$$\nabla^2 f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \dots & \dots & \frac{\partial^2 f}{\partial x_d^2} \end{pmatrix}$$

↓
Hessian

$$\Delta f = \nabla \cdot \nabla f$$

$$= \sum_{i=1}^d \frac{\partial^2}{\partial x_i^2} f(x)$$

In the heat equation, $p(\cdot)$ is the temperature, and $\Delta p(x)$ encodes the average difference in temperature between x and the neighborhood of x . This equation describes the diffusion of heat over time.

The Fokker-Planck Equation has both a drift and diffusion term. Also, as we see in Section 6 (pp. 29), we can absorb the diffusion term into the drift term via a time-varying vector field.

Sketch of proof of the FP Equation (for 1-d).

(Proof below adapted from [2]; see [1] for a complete proof).

Spcl case:
$$dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dB_t$$

$$\frac{\partial}{\partial t} P_t(z) = -\frac{\partial}{\partial z} (\mu(z, t) P_t(z)) + \frac{1}{2} \frac{\partial^2}{\partial z^2} \sigma^2(z, t) P_t(z)$$

Let $c(\cdot)$ be any bounded, differentiable function (assume existence of higher derivatives as needed).

Then,
$$\frac{\partial}{\partial t} E[c(X_t)]$$

$$\stackrel{h \text{ small}}{\approx} \frac{1}{h} E[c(X_{t+h}) - c(X_t)]$$

from approx. of
SDE, (1), p. 5

$$\approx \frac{1}{h} E \left[c \left(X_t + \mu(X_t, t) \cdot h + \sigma(X_t, t) \cdot (B_{t+h} - B_t) \right) - c(X_t) \right]$$

Taylor's Thm:
$$c(x + \delta_1 + \delta_2) \approx c(x) + c'(x) \cdot \delta_1 + c'(x) \cdot \delta_2 + c''(x) \cdot \frac{\delta_1^2}{2} + c''(x) \cdot \frac{\delta_2^2}{2} + c''(x) \delta_1 \delta_2 + \text{cubic terms.}$$

$$\approx \frac{1}{h} E \left[\begin{aligned} & \cancel{c(x_t)} + \cancel{c'(x_t) \mu(x_t, t) \cdot h} + \cancel{c'(x_t) \sigma(x_t, t) (B_{t+h} - B_t)} \\ & \underbrace{c''(x_t) h \cdot \mu(x_t, t)}_{\sigma_t^2 (B_{t+h} - B_t)} + \underbrace{\frac{c''(x_t) \cdot \mu^2(x_t, t) h^2}{2}}_{\approx 0} + \underbrace{\frac{c''(x_t) \sigma^2(x_t, t) (B_{t+h} - B_t)^2}{2}}_{E[\cdot] = h, \text{ indep increment}} \end{aligned} \right] - \cancel{c(x_t)}$$

$E[\cdot] = 0$

$E[\cdot] = 0$

$\alpha(h) \approx 0$

$E[\cdot] = h, \text{ indep increment}$

$\Rightarrow E[F(x_t) (B_{t+h} - B_t)^2]$

$= E[F(x_t)] \cdot h$

$$\approx \frac{1}{h} E \left[\cancel{c'(x_t) \mu(x_t, t) \cdot h} + \frac{c''(x_t) \sigma^2(x_t, t)}{2} \cdot \cancel{h} \right]$$

By tightening up and taking appropriate limit as $h \rightarrow 0$,

$$\frac{\partial}{\partial t} E[c(x_t)] = E \left[c'(x_t) \mu(x_t, t) + \frac{c''(x_t) \sigma^2(x_t, t)}{2} \right]$$

Expanding the expectations, we have

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} c(z) p_t(z) dz =$$

$$\int_{-\infty}^{\infty} \left(c'(z) \mu(z, t) + c''(z) \frac{\sigma^2(z, t)}{2} \right) p_t(z) dz$$

Now, we have:

$$(a) \quad \frac{\partial}{\partial t} \int_{-\infty}^{\infty} c(z) p_t(z) dz = \int_{-\infty}^{\infty} c(z) \frac{\partial}{\partial t} p_t(z) dz.$$

$$(b) \quad \int_{-\infty}^{\infty} \underbrace{c'(z)}_{u'} \underbrace{\mu(z, t) p_t(z)}_v dz = \underbrace{c(z)}_u \underbrace{\mu(z, t) p_t(z)}_v \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \underbrace{c(z)}_u \cdot \frac{\partial}{\partial z} \underbrace{(\mu(z, t) p_t(z))}_v dz.$$

Integration by parts

$$\int_a^b u(z) v'(z) dz = u(z) v(z) \Big|_a^b - \int_a^b u'(z) v(z) dz.$$

Now assume random variables are proper $\forall t$: Then

$$p_t(\infty) = p_t(-\infty) = 0 \quad \forall t.$$

$$\therefore c(z) \mu(z, t) p_t(z) \Big|_{-\infty}^{\infty} = 0.$$

$$\Rightarrow \int_{-\infty}^{\infty} c'(z) u(z, t) p_t(z) dz = \int_{-\infty}^{\infty} c(z) \left(-\frac{\partial}{\partial z} (u(z, t) p_t(z)) \right) dz$$

$$\begin{aligned} \textcircled{c} \quad \frac{1}{2} \int_{-\infty}^{\infty} \underbrace{c'(z)}_{v'} \underbrace{\sigma^2(z, t)}_u p_t(z) dz &= \left. \frac{1}{2} \underbrace{\sigma^2(z, t)}_u \underbrace{p_t(z)}_v \cdot \underbrace{c'(z)}_{u'} \right|_{-\infty}^{\infty} \xrightarrow{\text{to } 0} \\ &- \frac{1}{2} \int_{-\infty}^{\infty} \underbrace{c'(z)}_{v'} \cdot \underbrace{\frac{\partial}{\partial z} (\sigma^2(z, t) p_t(z))}_{u'} dz \end{aligned}$$

Next,

$$\int_{-\infty}^{\infty} \underbrace{c'(z)}_{v'} \underbrace{\frac{\partial}{\partial z} (\sigma^2(z, t) p_t(z))}_u dz$$

$$= \left. c(z) \cdot \frac{\partial}{\partial z} (\sigma^2(z, t) p_t(z)) \right|_{-\infty}^{\infty}$$

$$- \int_{-\infty}^{\infty} c(z) \frac{\partial^2}{\partial z^2} (\sigma^2(z, t) p_t(z)) dz.$$

Assume further: $\frac{\partial}{\partial z} \sigma^2(z, t) p_t(z) = 0$ at

$z = -\infty, \infty$

essentially means that $\frac{\partial}{\partial z} p_t(-\infty) = \frac{\partial}{\partial z} p_t(\infty) = 0$

(a stronger condition than properness, but is reasonable)

$$\begin{aligned} \therefore \frac{1}{2} \int_{-\infty}^{\infty} c''(z) \sigma^2(z, t) p_t(z) dz \\ = \frac{1}{2} \int_{-\infty}^{\infty} c(z) \frac{\partial^2}{\partial z^2} (\sigma^2(z, t) p_t(z)) dz \end{aligned}$$

Substituting (a), (b), (c) in (*),

$$\begin{aligned} \int_{-\infty}^{\infty} c(z) \left(\frac{\partial}{\partial t} p_t(z) \right) dz &= \int_{-\infty}^{\infty} c(z) \left(- \frac{\partial}{\partial z} (\mu(z, t) p_t(z)) \right) dz \\ &+ \int_{-\infty}^{\infty} c(z) \left(\frac{1}{2} \frac{\partial^2}{\partial z^2} (\sigma^2(z, t) p_t(z)) \right) dz \end{aligned}$$

Since above is true for all "reasonable" $c(z)$

we have

$$\frac{\partial}{\partial t} p_t(z) = - \frac{\partial}{\partial z} (\mu(z, t) p_t(z)) + \frac{1}{2} \frac{\partial^2}{\partial z^2} (\sigma^2(z, t) p_t(z))$$

This is the 1-d FP Equation



Aside:

Note also that the formal proof is different, and uses Dynkin's formula using Ito calculus

Theorem 7.4.1 (Dynkin's formula).

Let $f \in C_0^2(\mathbf{R}^n)$. Suppose τ is a stopping time, $E^x[\tau] < \infty$. Then

$$E^x[f(X_\tau)] = f(x) + E^x\left[\int_0^\tau Af(X_s)ds\right]. \quad (7.4.1)$$

← Øksendal, Chap 7:

A is the generator of the Markov Process

See Øksendal, prob. 8.3 for details.

8.3. (Kolmogorov's forward equation)

(aka Fokker-Planck Equation)

Let X_t be an Itô diffusion in $\mathbf{R}^n$ with generator

$$Af(y) = \sum_{i,j} a_{ij}(y) \frac{\partial^2 f}{\partial y_i \partial y_j} + \sum_i b_i(y) \frac{\partial f}{\partial y_i}; \quad f \in C_0^2$$

and assume that the transition measure of X_t has a density $p_t(x, y)$, i.e. that

$$E^x[f(X_t)] = \int_{\mathbf{R}^n} f(y) p_t(x, y) dy; \quad f \in C_0^2. \quad (8.6.34)$$

Assume that $y \rightarrow p_t(x, y)$ is smooth for each t, x . Prove that $p_t(x, y)$ satisfies the Kolmogorov forward equation

$$\frac{d}{dt} p_t(x, y) = A_y^* p_t(x, y) \quad \text{for all } x, y, \quad (8.6.35)$$

where A_y^* operates on the variable y and is given by

$$A_y^* \phi(y) = \sum_{i,j} \frac{\partial^2}{\partial y_i \partial y_j} (a_{ij} \phi) - \sum_i \frac{\partial}{\partial y_i} (b_i \phi); \quad \phi \in C^2 \quad (8.6.36)$$

(i.e. A_y^* is the adjoint of A_y .)

(Hint: By (8.6.34) and Dynkin's formula we have

$$\int_{\mathbf{R}^n} f(y) p_t(x, y) dy = f(x) + \int_0^t \int_{\mathbf{R}^n} A_y f(y) p_s(x, y) dy ds; \quad f \in C_0^2.$$

Now differentiate w.r.t. t and use that

$$\langle A\phi, \psi \rangle = \langle \phi, A^* \psi \rangle \quad \text{for } \phi \in C_0^2, \psi \in C^2,$$

where $\langle \cdot, \cdot \rangle$ denotes inner product in $L^2(dy)$.

(Note: The Dynkin's formula is the analog of the fundamental theorem of calculus for diffusions.)

Remark: We will revisit the FP Equation and connect it to the adjoint of the semigroup

generator of the Markov Process: $\frac{\partial}{\partial t} \pi_t^* = \mathcal{L}^* \pi_t^*$.
adjoint of the M.P. generator.

Scalar FP Equation: $\frac{\partial}{\partial t} p_t(z) = -\frac{\partial}{\partial z} (\mu(z,t) p_t(z)) + \frac{1}{2} \frac{\partial^2}{\partial z^2} \sigma^2(z,t) p_t(z)$

③ Density evolution for the Langevin Dynamics:

$$dX_t = \nabla \ln \pi^*(x_t) dt + \sqrt{2} dB_t, \quad X_t \in \mathbb{R}^d$$

$p_t(\cdot)$ is the density at time t ; $X_0 \sim p_0(\cdot)$

The FP Equation (for $d=1$).

$$\begin{aligned} \frac{\partial}{\partial t} p_t(z) &= -\frac{\partial}{\partial z} \left(\frac{\partial \ln \pi^*(z)}{\partial z} \cdot p_t(z) \right) \\ &\quad + \frac{1}{2} \frac{\partial^2}{\partial z^2} \cdot 2 \cdot p_t(z). \end{aligned}$$

Steady state: $\frac{\partial}{\partial t} p_t(z) = 0$.

$$\Rightarrow \frac{\partial^2}{\partial z^2} p_\infty(z) = \frac{\partial}{\partial z} \left(\frac{\partial \ln \pi^*(z)}{\partial z} \cdot p_\infty(z) \right).$$

Claim: $p_{\infty}(z) = \pi^*(z)$. Substitute and check:

$$\text{LHS} = \frac{\partial^2}{\partial z^2} \pi^*(z).$$

$$\text{RHS} = \frac{\partial}{\partial z} \left(\frac{1}{\cancel{\pi^*(z)}} \frac{\partial}{\partial z} \pi^*(z) \cdot \cancel{\pi^*(z)} \right) = \frac{\partial^2}{\partial z^2} \pi^*(z).$$



i.e., the invariant measure μ associated with the Langevin Dynamics is $\pi^*(\cdot)$.