

# Lecture 10: Forward and Backward equations for SDEs

## Readings

Recommended:

- Pavliotis [2014] 2.2-2.6, 3.4, 4.1-4.2
  - Gardiner [2009] 5.1-5.3
- Other sections are recommended too – this is a great book to read (and own as a reference), and it is strongly suggested to start looking through it.

Optional:

- Oksendal [2005] 7.3, 8.1,
- Korolov and Sinai [2010] 21.3, 21.4

Consider the multidimensional SDE

$$dX_t = b(X_t, t)dt + \sigma(X_t, t)dW_t, \quad X_t, W_t \in \mathbb{R}^d. \quad (1)$$

We have studied how to solve for solutions to (1), both analytically and numerically. But sometimes we don't want to study individual trajectories; rather, we want to study statistical properties of ensembles of trajectories. Such questions can be studied using partial differential equations associated with each SDE, an approach we follow in this and in following lectures.

We start with an important observation: *solutions to (1) are Markov processes*. We won't prove this, but rather point out that it is a natural consequence of the fact that increments  $X_t - X_s = \int_s^t b(X_u, u)du + \int_0^t \sigma(X_u, u)dW_u$  can be calculated using only  $(X_u)_{s \leq u < t}$ , and do not require knowing  $\{X_u\}_{u < s}$ . In fact, a stronger result holds, which is that solutions to (1) satisfy the Strong Markov property.

Because  $X$  is a Markov process, we can describe its time-evolution by a transition density  $p(x, t|y, s)$ , which is a function defined such that for any event  $A \subset \mathbb{R}^d$ ,

$$P(X_t \in A | X_s = y) = \int_A p(x, t|y, s)dx. \quad (2)$$

Formally, we may write  $p(x, t|y, s)dx = P(X_t \in [x, x + dx] | X_s = y)$ . Clearly, by definition we must have that  $p$  is nonnegative, integrable in  $x$ , and furthermore that

$$p(x, t|y, t) = \delta(x - y). \quad (3)$$

We'll also usually have that  $p$  satisfies other nice properties such as sufficient differentiability in its four arguments provided  $s \neq t$ .

From the transition density we can express the expectation of any function  $f(X_t)$  given  $X_s = y$  as

$$u(y, s) = \mathbb{E}^{y, s} f(X_t) = \int f(x)p(x, t|y, s)dx. \quad (4)$$

We can also compute the probability density  $\rho(x, t)$  of  $X_t$  at time  $t$ , given an initial density  $X_0 \sim \rho_0$ , as

$$\rho(x, t) = \int p(x, t|z, 0)\rho_0(z)dz. \quad (5)$$

Both  $u$  and  $\rho$  are functions from  $\mathbb{R}^d \times [0, \infty) \rightarrow \mathbb{R}$ .

We will derive evolution equations for  $u$  in (4) and  $\rho$  in (5), which will be the analogue of the Kolmogorov forward and backward equations we found for continuous time Markov chains. A tool for deriving such equations will be the Chapman-Kolmogorov equations (see Lecture 6):

$$p(y, t|x, s) = \int p(y, t|z, u)p(z, u|x, s)dz, \quad s < u < t. \quad (6)$$

To derive the Kolmogorov equations we'll make a number of assumptions on the functions involved. In particular, unless stated otherwise we'll assume that

- (i)  $b, \sigma$  are Lipschitz continuous and satisfy linear growth conditions at infinity;
- (ii) The diffusion tensor  $a(x) = \frac{1}{2}\sigma(x)\sigma^T(x)$  is *uniformly elliptic* on its domain  $D = \mathbb{R}^d$ : there is a constant  $\lambda_0 > 0$  such that

$$y^T a(x)y \geq \lambda_0 \quad \text{for all } y \in \mathbb{R}^d, x \in D. \quad (7)$$

In other words, the minimum eigenvalue of  $a(x)$  is bounded below by  $\lambda_0$ , uniformly in  $\mathbb{R}^d$ .

- (iii) Any function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  involved in the definition of  $u$  in (4) is in  $C^2(\mathbb{R}^d)$  and satisfies

$$f, \partial_i f, \partial_{ij} f \quad \text{are bounded and continuous.} \quad (8)$$

Some of these assumptions are stronger than one needs for the results below to be true, but proving them without these assumptions involves significant technical detail that is beyond the scope of this course (e.g. Durrett [1996]).

## 10.1 Generator of a time-homogeneous diffusion

Consider a time-homogeneous process  $X$  solving (1), and a function  $f$  satisfying (8). Applying Itô's formula to  $f(X_t)$  and integrating from  $s$  to  $t$  gives

$$f(X_t) - f(X_s) = \int_s^t \left( b(X_u) \cdot \nabla f(X_u) + \frac{1}{2} \sigma(X_u) \sigma^T(X_u) : \nabla^2 f(X_u) \right) du + \int_s^t \nabla f(X_u)^T \sigma(X_u) dW_u,$$

Take the expectation conditional on  $X_s = y$ ; written  $\mathbb{E}[f(X_t)|X_s = y] = \mathbb{E}^{y,s} f(X_t)$ :

$$\mathbb{E}^{y,s} f(X_t) - f(y) = \mathbb{E}^{y,s} \int_s^t \mathcal{L} f(X_u) du, \quad (9)$$

where the linear operator  $\mathcal{L}$  is defined by

$$(\mathcal{L} f)(x) = b(x) \cdot \nabla f(x) + a(x) : \nabla^2 f(x) \quad (10)$$

with

$$a(x) = \frac{1}{2} \sigma(x) \sigma^T(x).$$

**Definition.** The *generator* of a time-homogeneous diffusion process of the form (1) is the linear operator  $\mathcal{L}$ , defined in (10).

The generator  $\mathcal{L}$  is exactly analogous to the infinitesimal generator of a continuous-time Markov chain. Recall that for a time-homogeneous, continuous-time Markov chain, we defined the generator to be the matrix  $Q$  such that, for all suitable functions  $f$ ,

$$\lim_{t \rightarrow 0^+} \frac{\mathbb{E}^x f(X_t) - f(x)}{t} = (Q\mathbf{f})_x,$$

where  $\mathbf{f} = (f(x))_{x \in S}$  is a vector,  $\mathbb{E}^x = \mathbb{E}^{x,0}$ , and  $(Q\mathbf{f})_x$  equals the vector  $Q\mathbf{f}$  evaluated at component  $x$ . The generator was a linear operator acting on a finite- or countable-dimensional vector space.

Consider the same calculation for a time-homogeneous diffusion process. Over infinitesimal time intervals, the expectation evolves as, using (9),

$$\begin{aligned} \lim_{t \rightarrow 0^+} \frac{\mathbb{E}^{x,0} f(X_t) - f(x)}{t} &= \lim_{t \rightarrow 0^+} \mathbb{E}^x \frac{1}{t} \int_0^t \mathcal{L}f(X_u) du \\ &= \mathbb{E}^x \lim_{t \rightarrow 0^+} \frac{1}{t} \int_0^t \mathcal{L}f(X_u) du && \text{(Dominated Convergence Theorem)} \\ &= \mathbb{E}^x \mathcal{L}f(X_0) && \text{(Mean value theorem)} \\ &= (\mathcal{L}f)(x). \end{aligned}$$

The generator  $\mathcal{L}$  is now a linear operator which acts on functions, a continuous generalization of a matrix which acts on vectors.

*Remark.* In the probability literature the generator of a time-homogeneous diffusion process is *defined* to be the operator  $\mathcal{A}$  acting on functions  $f \in L^\infty$  given by

$$\mathcal{A}f(x) = \lim_{t \rightarrow 0^+} \frac{\mathbb{E}^x f(X_t) - f(x)}{t} \quad (11)$$

whenever the limit exists. When  $f$  is sufficiently smooth the limit equals  $\mathcal{L}f$  as in (10). However, the limit can exist for a broader set of functions. The *domain* of the generator  $\mathcal{A}$ , written  $D(\mathcal{A})$ , is the set of  $f \in L^\infty$  for which the limit above exists in the  $L^\infty$  norm.

*Remark.* The coefficients of the operator  $\mathcal{L}$  can be obtained from the moments of the diffusion process, as

$$b_i(x) = \lim_{t \rightarrow 0} \frac{\mathbb{E}^x[(X_t)_i - x_i]}{t}, \quad a_{ij}(x) = \lim_{t \rightarrow 0} \frac{\mathbb{E}^x[(X_t)_i - x_i][(X_t)_j - x_j]}{t}.$$

See e.g. Gardiner [2009], Pavliotis [2014], Karlin and Taylor [1981].

## 10.2 Backward Kolmogorov equation

The first use of the generator is in the backward equation.

**Backward Kolmogorov Equation** (Time-homogeneous). Let  $X$  solve a time-homogeneous SDE (1). Let  $f$  satisfy (8) and define

$$u(x, t) = \mathbb{E}^x f(X_t) = \mathbb{E}[f(X_t) | X_0 = x]. \quad (12)$$

Then for  $t \geq 0$ ,  $u$  satisfies

$$\partial_t u = \mathcal{L}u, \quad u(x, 0) = f(x). \quad (13)$$

*Remark.* For a continuous-time Markov chain, the vector  $u(t)$  defined as in (12) evolves as  $\frac{du}{dt} = Qu$ , which is the discrete version of (13).

*Proof.* Showing that the function  $u$  defined by (12) satisfies (13) is technical, as it requires showing that  $u$  has two derivatives in  $x$  and one derivative in  $t$  (e.g. Durrett [1996], Section 7). Instead, we show that if  $u$  is a bounded solution to (13), then  $u$  satisfies (12) (Varadhan [2007], p.95-96). We show this for a scalar SDE but a multidimensional one follows in the same way.

Let  $t$  be fixed and let  $Z_s = u(X_s, t - s)$ . From Itô's formula we have (all functions below are evaluated at  $(X_s, t - s)$ )

$$\begin{aligned} dZ_s &= -u_t ds + u_x dX_s + au_{xx} ds \\ &= (-u_t + bu_x + au_{xx}) ds + u_x \sigma dW_s = u_x \sigma dW_s, \end{aligned}$$

since  $u$  solves the PDE, by assumption. Therefore

$$Z_s = Z_0 + \int_0^s u_x(X_r, t - r) \sigma(X_r) dW_r.$$

Taking expectations shows that  $\mathbb{E}^x Z_s = \mathbb{E}^x Z_0$  for all  $0 \leq s \leq t$ , and using the initial condition of the PDE shows that  $\mathbb{E}^x Z_t = \mathbb{E}^x u(X_t, 0) = \mathbb{E}^x f(X_t)$ . Putting this together gives

$$\mathbb{E}^x f(X_t) = \mathbb{E}^x Z_t = \mathbb{E}^x Z_0 = u(x, t),$$

which is what we wish to show. □

An alternate derivation was shown in Lecture 6, using the abstract semigroup operator  $T_t f(x) := \mathbb{E}^{x,0} f(X_t)$  and the Chapman-Kolmogorov equations.

The proof of the backward equation shows that solutions to an SDE, can be thought of as characteristics for a PDE. When  $\sigma = 0$  so that (1) is a deterministic equation, the backward equation is the first-order PDE  $\partial_t u = b(x) \cdot \nabla u$ . Then (1) is the equation that the characteristics for the PDE must satisfy,<sup>1</sup> and our proof showed the solution  $u(x, t)$  to the PDE (13) is constant on characteristics. When we have noise,  $\sigma \neq 0$ , then the solutions to the PDE (13) no longer has deterministic characteristics, but rather it has noisy characteristics, solving (1). The solution can be expressed as the average of  $f$ , averaged over the ensemble of characteristics with a given starting point.

<sup>1</sup>Actually the characteristics would satisfy  $\frac{dx}{ds} = -b(x)$ , but we prefer to think about integrating the SDE forward in time, and then integrating backwards along the characteristic to get the solution  $u$ .

**Example 10.1** (Brownian motion) Consider a Brownian motion, which solves the SDE  $dX_t = dW_t$ . The generator is  $\mathcal{L} = \frac{1}{2}\partial_{xx}$  so the backward equation is

$$\partial_t u = \frac{1}{2}\partial_{xx}u, \quad u(x, 0) = f(x).$$

This is a heat equation for  $u$ , with initial condition  $f(x)$ . Therefore, we can solve for the evolution of statistics such as  $\mathbb{E}^x X_t$ ,  $\mathbb{E}^x X_t^2$ , etc, (or rather bounded versions of these functions), by solving the heat equation with an appropriate initial condition.

As for Markov chains, the backward equation is called backward because for a time-inhomogeneous process, we must solve a PDE backward in time.

**Backward Kolmogorov Equation** (Time-inhomogeneous). *Let  $X$  solve SDE (1). Let  $f$  satisfy (8) and define*

$$u(y, s) = \mathbb{E}^{y, s} f(X_t) = \mathbb{E}[f(X_t) | X_s = y]. \quad (14)$$

Then  $u$  solves

$$\partial_s u(y, s) + \mathcal{L}u(y, s) = 0, \quad s < t, \quad u(y, t) = f(y), \quad (15)$$

where  $\mathcal{L}$  is defined as in (10) but with time-dependent coefficients:

$$(\mathcal{L}f)(x, t) = b(x, t) \cdot \nabla f(x) + a(x, t) : \nabla^2 f(x). \quad (16)$$

**Exercise 10.1.** Show (15), by defining  $Z_s = u(X_s, s)$  and proceeding as in the proof of the time-homogeneous backward equation.

**Exercise 10.2.** Derive the backward equation (13) for a time-homogeneous process, from the backward equation (17) for a time-inhomogeneous process, by considering the function  $v(x, s) = u(x, t - s)$ .

There is a link between the Green's function for the inhomogeneous backward equation, and the transition density for the stochastic process. Applying  $\partial_s, \mathcal{L}$  to the right-hand side of (4) gives

$$\int f(x) (\partial_s p(x, t | y, s) + \mathcal{L}_y p(x, t | y, s)) dx = 0,$$

where the operator  $\mathcal{L}_y$  acts on the  $y$ -variables of  $p$ . Since this holds for all test functions  $f$ , we obtain a version of the backward equation for the transition density.

**Backward Kolmogorov Equation** (transition density). *The transition density  $p(x, t | y, s)$  evolves jointly in  $y, s$  as*

$$\partial_s p + \mathcal{L}_y p = 0, \quad s < t, \quad p(x, t | y, t) = \delta(x - y), \quad (17)$$

where  $\mathcal{L}_y$  acts on the  $y$ -variable of  $p$ .

Hence, the transition density solves the inhomogeneous backward equation in the  $y, s$  variables, with a point source initial condition. In fact, the transition density is the Green's function for the inhomogeneous backward equation.

**Example 10.2** A Brownian motion has transition density

$$p(x, t | y, s) = \frac{1}{\sqrt{2\pi(t-s)}} e^{-\frac{(x-y)^2}{2(t-s)}},$$

which one can verify solves (17).

## 10.3 Forward Kolmogorov equation (Fokker-Planck equation)

### 10.3.1 Derivation of the Fokker-Planck equation

Now we consider the forward equation, known in physics communities as the *Fokker-Planck equation*. It will be formulated in terms of  $\mathcal{L}^*$ , the formal adjoint of  $\mathcal{L}$ . This is the operator that satisfies

$$\langle \mathcal{L}f, g \rangle = \langle f, \mathcal{L}^*g \rangle \quad (18)$$

for all  $f, g$  in suitable function spaces, and where  $\langle f, g \rangle = \int_{\mathbb{R}^d} fg dx$  is the  $L^2$ -inner product. (Which function spaces  $f, g$  live in is part of the definitions of  $\mathcal{L}, \mathcal{L}^*$ , as we'll see in Section 10.4.) Let's work out the formal expression for  $\mathcal{L}^*$ . We have

$$\begin{aligned} \langle \mathcal{L}f, g \rangle &= \int g(b \cdot \nabla f + a : \nabla^2 f) dx \\ &= \int \left( \nabla \cdot (fgb) - f \nabla \cdot (gb) + \nabla \cdot (ga \cdot \nabla f) - \nabla \cdot (f \nabla \cdot (ga)) + f \nabla \cdot \nabla \cdot (ga) \right) dx \\ &= \int f \left( -\nabla \cdot (bg) + \nabla \cdot \nabla \cdot (ag) \right) dx + \int \left( \nabla \cdot (fgb) + \nabla \cdot (ga \cdot \nabla f) - \nabla \cdot (f \nabla \cdot (ga)) \right) dx. \end{aligned}$$

If the terms  $g(a \cdot \nabla f)$ ,  $f(gb - \nabla \cdot (ga))$  vanish sufficiently quickly at infinity, then the last integral vanishes by the divergence theorem, and we obtain the adjoint operator as

$$\mathcal{L}^*g(x, t) = -\nabla \cdot (b(x, t)g(x)) + \nabla \cdot \nabla \cdot (a(x, t)g(x)). \quad (19)$$

*Remark.* For a Markov chain with generator  $Q$ , the above calculation asks for the matrix  $Q^*$  such that  $\langle Qx, y \rangle = \langle x, Q^*y \rangle$  for all vectors  $x, y$ . But we have

$$\langle Qx, y \rangle = y^T Qx = x^T Q^T y = \langle x, Q^T y \rangle,$$

and hence  $Q^* = Q^T$ . The adjoint in an infinite-dimensional vector space generalises the concept of transpose in a finite-dimensional vector space.

The adjoint operator appears in the forward equation, also known as the Fokker-Planck equation, which is the same equation whether the process is time-homogeneous or not.

**Forward Kolmogorov Equation** (Fokker-Planck equation). *Let  $\rho(x, t)$  be the probability density of  $X_t$  at time  $t$ , and let  $\rho_0(x)$  be its initial probability density. Then provided  $\rho \in C^{2,1}(\mathbb{R}^d \times \mathbb{R}^+)$  ( $\rho$  is twice continuously differentiable in  $x$  and once continuously differentiable in  $t$ ),  $\rho$  solves*

$$\partial_t \rho = \mathcal{L}^* \rho \quad (t > 0), \quad \rho(x, 0) = \rho_0(x), \quad (20)$$

where operator  $\mathcal{L}^*$  is defined in (19).

*Remark.* For a continuous-time Markov chain, the probability distribution  $\mu(t)$  evolved as  $\frac{d\mu}{dt} = \mu Q^T \Leftrightarrow \frac{d\mu^T}{dt} = Q^T \mu^T$ . This is the discrete version of (20), since for a finite-dimensional, real operator, the adjoint of the generator is  $Q^* = Q^T$ .

*Proof.* Let  $f$  be a function satisfying (8), let  $T > 0$ , and let  $u(x, t) = \mathbb{E}^{x,t} f(X_T)$  for  $0 \leq t \leq T$  as in the inhomogeneous backward equation, (14). We may establish that

$$\int u(x, t) \rho(x, t) dx = \mathbb{E}^{\rho_0} f(X_T), \quad (21)$$

which notably is independent of  $t$ . To show (21) in detail, we calculate:

$$\begin{aligned} \int u(x, t) \rho(x, t) dx &= \int f(y) p(y, T | x, t) p(x, t | z, 0) \rho_0(z) dx dy dz \\ &= \int f(y) p(y, T | z, 0) \rho_0(z) dz dy = \mathbb{E}^{\rho_0} f(X_T), \end{aligned}$$

by Fubini's theorem, and the Chapman-Kolmogorov equations (6).

Taking a time derivative of (21) and moving it into the integral (assuming this is possible), gives

$$\begin{aligned} 0 &= \frac{\partial}{\partial t} \int u(x, t) \rho(x, t) dx = \int \rho \partial_t u dx + \int u \partial_t \rho dx \\ &= \int \rho (-\mathcal{L}u) dx + \int u \partial_t \rho dx \\ &= \int u (-\mathcal{L}^* \rho + \partial_t \rho) dx. \end{aligned}$$

Taking  $T = t$  shows that

$$\int f(x) (-\mathcal{L}^* \rho(x, t) + \partial_t \rho(x, t)) dx = 0.$$

Since this holds for for all test functions  $f$ , we obtain (20).  $\square$

The Green's function for the forward equation is also the transition density  $p(x, t | y, s)$ , but this time evolving in the  $x, t$  variables. :

**Forward Kolmogorov Equation** (transition density). *The transition density  $p(x, t | y, s)$  evolves jointly in  $x, t$  as*

$$\partial_t p = \mathcal{L}_x^* p, \quad p(x, s | y, s) = \delta(x - y). \quad (22)$$

where  $\mathcal{L}_x$  acts on the  $x$ -variable of  $p$ .

**Exercise 10.3.** Argue why (22) should hold, from (20). You can assume that  $p$  has as many derivatives as you need.

**Example 10.3** (Brownian motion) For a Brownian motion solving  $dX_t = dW_t$ , we have  $\mathcal{L} = \frac{1}{2} \partial_{xx}$ , so  $\mathcal{L}^* = \frac{1}{2} \partial_{xx}$ . The probability density therefore solves a heat equation

$$\partial_t \rho = \frac{1}{2} \partial_{xx} \rho, \quad \rho|_{t=0} = \rho_0.$$

In this example we have  $\mathcal{L} = \mathcal{L}^*$  but this almost always won't be the case.

*Remark.* The forward equation is weaker than the backward equation – in general it is only expected to hold in a weak sense. Indeed, the forward equation requires taking derivatives of  $b, \sigma$ , but these are not required to be differentiable for the SDE to have a unique strong solution; their derivatives may only exist in a weak sense. See Evans [2010] for the construction of weak solutions to partial differential equations.

*Remark.* The Fokker-Planck equation for a Stratonovich SDE has a convenient form:

$$dX_t = \sigma(X_t) \circ dW_t \iff \partial_t \rho = \frac{1}{2} \sum_{i,j,k} \partial_i (\sigma_{ik} \partial_j (\sigma_{jk} \rho)) = \frac{1}{2} \nabla \cdot (\sigma \nabla \cdot (\sigma^T \rho)).$$

### 10.3.2 Physical interpretation of the Fokker-Planck equation

The Fokker-Planck equation has a physical interpretation in terms of the flux of probability. Write (20) as

$$\partial_t \rho + \nabla \cdot \underline{j} = 0, \quad \text{where} \quad \underline{j} = b(x,t)\rho - \nabla \cdot (a(x,t)\rho). \tag{23}$$

This is a conservation equation for the probability density  $\rho$ . The quantity  $\underline{j}$ , which tells us how probability moves, is called the *probability current*, or *probability flux*. This has an interpretation using fluid dynamics. Consider a passive tracer in a fluid, such as a particle of milk in a coffee cup that is being stirred. The particle will be advected by the fluid’s velocity, but it will also diffuse because of the random jiggling of the fluid molecules. Suppose

- $\rho(x,t)$  = concentration of a passive tracer
- $b(x,t)$  = velocity of fluid
- $a(x,t)$  = diffusion tensor in fluid

Then the Fokker-Planck equation says that the tracer is advected with velocity  $b$ , and diffuses with diffusion tensor  $a$ . Probability behaves exactly like a passive tracer in a fluid! <sup>2</sup>

From the probability flux, we can compute the total probability that crosses a surface  $S$  per unit time. To see how, consider a closed surface  $S$  with interior  $\Omega$ . The change in total probability in  $\Omega$  per unit time is, by the Divergence Theorem,

$$\frac{d}{dt} \int_{\Omega} \rho = \int_{\Omega} -\nabla \cdot \underline{j} = \int_S -\underline{j} \cdot \hat{n},$$



where  $\hat{n}$  is the unit outward normal. The flux across  $S$  is  $\int_S \underline{j} \cdot \hat{n}$ .

Choosing  $\Omega = \mathbb{R}^d$ , this calculation also shows that probability is conserved, provided  $j(x,t)$  decays sufficiently quickly as  $|x| \rightarrow \infty$ .

### 10.3.3 Existence of solutions to the Fokker-Planck equation

When does (20) have a solution? We clearly need  $\rho$  to be integrable, as it is a probability density. It turns out we have more control over  $\rho$  provided we make some assumptions on the functions involved.

We say that  $\rho$  is a *classical solution to (20)* if

<sup>2</sup>The more familiar equation for a passive tracer is  $\partial_t c + u \cdot \nabla c = [\text{diffusion}]$ , because for many fluids,  $\nabla \cdot u = 0$ .



- (i)  $\rho \in C^{2,1}(\mathbb{R}^d \times \mathbb{R}^+)$  and (20) holds for all  $t > 0$ ;  
(ii) for all  $T > 0$ , there exists constants  $C > 0, \alpha > 0$  such that

$$\sup_{0 \leq t \leq T} |\rho(x, t)| \leq Ce^{\alpha|x|^2}; \quad (24)$$

- (iii)  $\lim_{t \rightarrow 0} \rho(x, t) = \rho_0(x)$ .

The existence of a classical solution to (20) is best framed by writing  $\mathcal{L}^*$  in nondivergence form, as

$$\mathcal{L}^* \rho = a : \nabla^2 \rho + \tilde{b} \cdot \nabla \rho + c \rho,$$

where

$$\tilde{b} = -b + 2\nabla \cdot a, \quad c = -\nabla \cdot b + \nabla \cdot \nabla \cdot a.$$

**Theorem.** *If  $a$  is uniformly elliptic, with bounded coefficients:  $|a_{ij}(x)| \leq M$ , and furthermore if  $|\tilde{b}(x)| \leq M(1 + |x|)$ , and  $|c| \leq M(1 + |x|^2)$ , and  $|\rho_0(x)| \leq Ce^{\alpha|x|^2}$ , then there exists a unique classical solution to the Fokker-Planck equation (20). Furthermore, there exist constants  $K, \delta > 0$ , such that*

$$|\rho|, |\rho_t|, |\nabla \rho|, \|\nabla^2 \rho\| \leq Kt^{(-d+2)/2} e^{-\frac{1}{2t}\delta|x|^2} \quad (25)$$

for all  $t > 0$ .

See Pavliotis [2014], Ch. 4, and Friedman [2004].

This theorem shows that if we ask for a solution that doesn't grow too quickly, we actually end up with a probability density that is very well-behaved –  $\rho$  and many of its derivatives are bounded and integrable. In particular, (25) shows that we were justified in throwing out the boundary terms in our derivation of (19), since (remembering also the conditions (8) on  $f$ ), both terms  $\rho(a \cdot \nabla f)$  and  $f(\rho b - \nabla \cdot (\rho a))$  will decay rapidly enough at infinity that they will vanish when integrated over a large ball.

We also note that from the maximum principal for parabolic equations, we can show that  $\rho(x, t) \geq 0$  whenever  $\rho_0(x) \geq 0$ .

The condition (24) that solutions don't grow too quickly can be thought of as a kind of boundary condition for (20), required to ensure uniqueness. For example, for the heat equation  $\partial_t \rho = \Delta \rho$ ,  $\rho(x, 0) = 0$ , one can construct infinitely many solutions, however they all grow rapidly at infinity [John, 1978, Ch. 7].

## 10.4 Boundary conditions for the forward and backward equations

Often we are interested in stochastic processes that live in a bounded (open) domain  $\Omega \subset \mathbb{R}^d$  with boundary  $\partial\Omega$ . Examples include a bacteria navigating in a petri dish, an ion moving through an ion channel, a protein wiggling around inside a cell, micrometer colloidal particles in a microfluidic channel, a milk particle in a coffee cup, etc.

When the process hits the boundary, there are various things that could happen to it – it could be reflected, like a billiard ball, it could be absorbed, like a fly sticking to a fly trap, it could be reflected with some probability and otherwise absorbed, etc. All of these possibilities are captured at the level of the forward and backward equations, by imposing boundary conditions for these equations on  $\partial\Omega$ . We will variously refer

to boundary conditions for the forward or backward equation as boundary conditions for  $\mathcal{L}^*$  or  $\mathcal{L}$ . Each of these operators comes with a domain of definition,  $\mathcal{D}(\mathcal{L})$ ,  $\mathcal{D}(\mathcal{L}^*)$ , which are classes of functions on which each operator is assumed to act. These classes must be related to each other if (18) is to hold, because the boundary terms in the integration by parts must vanish.

Our approach to introducing boundary conditions will be to first list some possible boundary conditions for the forward equation, because it has a more physical interpretation, and then derive the corresponding boundary conditions for the backward equation.

A more direct approach would explicitly construct solutions to the SDE with the corresponding boundary behaviour, and then use the definition of the generator, (11), to determine the behaviour of the generator  $\mathcal{L}$  at the boundary, and then finally determine the boundary behaviour of  $\mathcal{L}^*$ . However, explicitly constructing solutions to SDEs with given boundary behaviour is a challenge that is beyond the scope of this course, though we will give insight into the origin of the boundary conditions at the level of trajectories in Section 10.4.3, by constructing a continuous-time Markov chain which approximates the solution to an SDE.

#### 10.4.1 Boundary conditions for the Forward Equation ( $\mathcal{L}^*$ )

Here are common boundary conditions for  $\mathcal{L}^*$ , each associated with different kinds of boundary behaviours. In what follows,  $\hat{n}$  always denotes an outward normal to a boundary.

- *Reflecting boundary*

$$\underline{j} \cdot \hat{n} = 0 \quad \text{on } \partial\Omega.$$

This corresponds to trajectories being reflected at the boundary. There is no net flux of probability across the boundary, so the total probability in the domain is conserved:  $\frac{d}{dt} \int_{\Omega} \rho = 0$ .

- *Absorbing boundary*

$$\rho = 0 \quad \text{on } \partial\Omega.$$

This corresponds to trajectories being absorbed at the boundary and taken out of the system immediately. The total probability is *not* conserved.

- *Periodic boundary* (on an interval  $[a, b]$ )

$$\underline{j}|_{b^-} = \underline{j}|_{a^+}, \quad \rho|_{b^-} = \rho|_{a^+}.$$

Trajectories that leave one side, immediately re-enter on the other. Total probability is conserved.

- *At a discontinuity* If the coefficients  $b(x, t)$ ,  $a(x, t)$  are discontinuous on some surface  $S$ , but particles can still cross it, then we actually have separate equations, one on each part of the domain where the coefficients are continuous. We “match” the solutions with the conditions that both the probability, and the normal components of the probability current, are continuous across  $S$

$$\underline{j} \cdot \hat{n}|_{S^+} = \underline{j} \cdot \hat{n}|_{S^-}, \quad \rho|_{S^+} = \rho|_{S^-}.$$

Note that the derivatives of  $\rho$  may not necessarily be continuous, even if the flux is. This boundary condition corresponds to trajectories that move freely from one part of the domain to another without reflection or adsorption; it conserves total probability.

**Example 10.4** Consider a colloidal particle in a two-dimensional domain  $\Omega = \{(x, z) : z > 0\}$ , which is advected horizontally by a shear flow  $u(x) = (z, 0)^T$ , moves downwards with constant velocity  $-b(0, 1)^T$  (for example due to gravity), and diffuses isotropically with diffusion coefficient  $D$ . The Fokker-Planck equation for the probability density of the particle is

$$\partial_t \rho = \partial_x(-z\rho) + \partial_z(b\rho) + D(\partial_{xx}\rho + \partial_{zz}\rho),$$

and hence the flux is

$$j(x, z, t) = \begin{pmatrix} z \\ -b \end{pmatrix} \rho(x, z, t) - D \begin{pmatrix} \partial_x \rho(x, z, t) \\ \partial_z \rho(x, z, t) \end{pmatrix}.$$

At the boundary  $\partial\Omega = \{(x, z) : z = 0\}$ , a reflecting boundary condition would be  $j \cdot \hat{n} = 0$  where  $\hat{n} = (0, -1)^T$ , and hence

$$b\rho + D\partial_z\rho = 0 \quad \text{at } z = 0.$$

#### 10.4.2 Boundary conditions for the backward equation ( $\mathcal{L}$ )

Boundary conditions for the backward equation, or for  $\mathcal{L}$ , can be derived from those for the forward equation, or  $\mathcal{L}^*$ , using integration by parts, by asking that (18) hold for all functions  $f, g$  satisfying the appropriate boundary conditions. Our calculations just after (18) showed that, formally,

$$\langle \mathcal{L}f, g \rangle = \langle f, \mathcal{L}^*g \rangle + \int_{\partial\Omega} f \underline{j} \cdot \hat{n} + g(a \cdot \nabla f) \cdot \hat{n}, \quad (26)$$

where  $\underline{j} = b(x, t)f - \nabla \cdot (a(x, t)g)$  (see (23)). We need the integral over  $\partial\Omega$  to vanish for all functions  $f \in \mathcal{D}(\mathcal{L})$ , i.e. functions satisfying the boundary conditions associated with  $\mathcal{L}$ , and for all  $g \in \mathcal{D}(\mathcal{L}^*)$ , i.e. functions satisfying the boundary conditions associated with  $\mathcal{L}^*$ . Given boundary conditions for one of these operators, we use the vanishing of the boundary terms to determine the corresponding boundary conditions for the other operator. Here are some examples:

- *Reflecting boundary.* The boundary condition for  $\mathcal{L}^*$  is  $j \cdot \hat{n} = 0$  on  $\partial\Omega$ . Therefore, the first term in the integrand in (26) is always zero, so we must only ensure the second term is zero. A condition that ensures this is

$$(a \cdot \nabla f) \cdot \hat{n} = 0 \quad \text{on } \partial\Omega.$$

In components,  $\sum_{i,j} n_i a_{ij} \partial_j f = 0$ .

- *Absorbing boundary.* The boundary condition for  $\mathcal{L}^*$  is  $g = 0$  on  $\partial\Omega$ , so the second term in the integrand in (26) is always zero. To ensure the first term is also zero, we must choose

$$f = 0 \quad \text{on } \partial\Omega.$$

The other conditions are left as exercises on the homework.

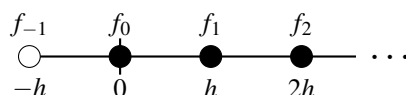
### 10.4.3 Boundary conditions from a limit of random walks\*

It is challenging to write down boundary conditions explicitly at the level of the SDE; doing so involves concepts such as local time which are beyond the scope of this course. One way to gain insight into the microscopic origin of the boundary conditions is to construct a continuous-time Markov chain which approximates the solution to the SDE, and then to see how this process behaves at the boundary of its domain. We illustrate with an example.

Consider a Brownian motion on  $[0, \infty)$ , with a reflecting boundary condition at 0. The generator is

$$\mathcal{L}f = \frac{1}{2} \partial_{xx} f \quad \partial f|_{x=0} = 0.$$

Let's discretize the domain of the process as  $\mathbb{R}^h = \{0, h, 2h, 3h, \dots\}$ , where  $h$  is the spacing between neighbouring grid points. We will construct a continuous-time Markov chain on  $\mathbb{R}^h$ , whose generator  $Q$  is an approximation to  $\mathcal{L}$ . Let  $f \in C_b^4(\mathbb{R})$ , and let  $f_0, f_1, \dots$  be the values of the function at the grid points, i.e.  $f_k = f(kh)$  as illustrated below.



The white dot is a ghost grid point, which we recruit in our construction. At each interior grid point,  $\mathcal{L}f$  can be approximated by

$$(\mathcal{L}f)(kh) = \frac{f_{k+1} - 2f_k + f_{k-1}}{2h^2} + O(h^2), \quad k \geq 1. \tag{27}$$

This approximation is a second-order centered finite difference approximation to the second derivative operator  $\partial_{xx}$ . At the boundary grid point,  $k = 0$ , we do not know the value of the ‘ghost’ point  $f_{-1}$  that is needed in (27), so we solve for it using the boundary condition. The discretized boundary condition is

$$\frac{f_1 - f_{-1}}{2h} + O(h^2) = 0 \quad \Leftrightarrow \quad f_{-1} = f_1 + O(h^3),$$

where again we used a second-order centered finite difference scheme to evaluate  $\partial_x f$ . Using this equation to eliminate  $f_{-1}$  in (27) with  $k = 0$  gives an approximation to the generator at the boundary as

$$(\mathcal{L}f)(0) = \frac{f_1 - 2f_0}{h^2} + O(h). \tag{28}$$

Now, we construct a continuous-time Markov chain  $Y_t$  with state space  $\mathbb{R}^h$ , whose generator  $Q$  is the discrete approximation to  $\mathcal{L}$ . That is, we set

$$(Qf)_k = \begin{cases} \frac{f_{k+1} - 2f_k + f_{k-1}}{2h^2}, & k = 1, 2, \dots, \\ \frac{f_1 - f_0}{h^2}, & k = 0. \end{cases} \tag{29}$$

From the generator we can read off how  $Y_t$  behaves in the interior points and at the boundary point; recall the Gillespie algorithm from Lecture 4. At an interior point,  $k > 0$ ,  $Y_t$  jumps left or right with equal probability,

with a holding time  $\tau_k \sim \text{Exp}(1/h^2)$  whose average is  $\mathbb{E}\tau_k = h^2$ . At a boundary point,  $k = 0$ ,  $Y_t$  jumps to the right, with a holding time  $\tau_0 \sim \text{Exp}(1/h^2)$  whose average is  $\mathbb{E}\tau_0 = h^2$ . Therefore, whenever  $Y_t$  hits zero its next step is to the right; it is “reflected” from the boundary.

Now consider the same discretization but for the absorbing boundary condition,  $f|_{x=0} = 0$ . The discretized generator is

$$(Qf)_k = \begin{cases} \frac{f_{k+1} - 2f_k + f_{k-1}}{2h^2}, & k = 1, 2, \dots, \\ 0, & k = 0. \end{cases} \quad (30)$$

Now, when  $Y_t$  hits 0, it stays there forever. It is “absorbed” at the boundary point.

You can repeat this discretization for a more general process with generator (10), to justify boundary conditions for the backward equation. For more details on how to approximate SDEs using continuous-time Markov chains, see Bou-Rabee and Vanden-Eijnden [2018], and for the extension to boundary conditions, see Bou-Rabee and Holmes-Cerfon [2019].

## 10.5 Stationary distribution

Suppose the SDE (1) is time-homogeneous. Is there a probability density that doesn’t change with time? Recall that a stationary distribution for a continuous-time Markov chain is a probability distribution  $\pi$  such that  $\pi = \pi P(t)$  for all  $t \geq 0$ . The definition is the same for a diffusion process.

**Definition.** A *stationary distribution* or *invariant measure* is a probability distribution  $\mu(x)$  that doesn’t change with time, i.e. such that

$$P(X_t \in A | X_0 \sim \mu(x)) = \mu(A) = \int_{x \in A} \mu(dx) \quad (31)$$

for all measurable sets  $A \subset \mathbb{R}^d$ . If the process has a probability density  $\rho$ , then  $\rho$  is a *stationary density* if  $\partial_t \rho = 0$ , so that

$$\mathcal{L}^* \rho = 0. \quad (32)$$

Explicitly, a stationary density  $\rho$  solves the elliptic PDE

$$\nabla \cdot \mathbf{j} = 0 \iff \nabla \cdot (b(x)\rho - \nabla \cdot (a(x)\rho)) = 0. \quad (33)$$

**Example 10.5** (Brownian motion) Suppose we have a one-dimensional Brownian motion on the interval  $[0, 1]$  with reflecting boundary conditions. The stationary distribution solves the equation

$$\rho_{xx} = 0, \quad \rho_x|_{x=0} = \rho_x|_{x=1} = 0.$$

Integrate twice to find  $\rho(x) = A + BX + Cx^2$  for some constants  $A, B, C$ . Using the boundary conditions shows that  $\rho(x) = \text{const}$ . Using the fact that  $\int_0^1 \rho(x) dx = 1$  since  $\rho$  is a probability density, shows that  $\rho(x) = 1$ . The stationary distribution is constant – there is equal probability of finding a Brownian motion anywhere in its domain.

**Exercise 10.4.** Show that the stationary distribution of a Brownian motion with reflecting boundary conditions in any bounded domain  $\Omega \subset \mathbb{R}^d$ , is constant in that domain.

**Example 10.6** (Ornstein-Uhlenbeck process) Consider  $dX_t = -\alpha X_t + \sigma dW_t$ . The stationary distribution solves

$$\alpha \frac{\partial}{\partial x}(x\rho) + \frac{1}{2}\sigma^2 \frac{\partial^2 \rho}{\partial x^2} = 0.$$

Let's look for a solution with  $\underline{j} = 0$ . Then we must solve

$$\alpha x\rho + \frac{1}{2}\sigma^2 \rho_x = 0 \quad \Rightarrow \quad \frac{\rho_x}{\rho} = -\frac{2\alpha x}{\sigma^2} \quad \Rightarrow \quad \ln \rho = -\frac{\alpha}{\sigma^2}x^2 + C$$

where  $C$  is a constant. The stationary distribution is

$$\rho = \frac{1}{\sqrt{2\pi\sigma^2/(2\alpha)}} e^{-\frac{1}{2}\frac{x^2}{\sigma^2/(2\alpha)}}.$$

This shows the stationary distribution is Gaussian, with mean 0, variance  $\sigma^2/2\alpha$ .

**Example 10.7** (Brownian dynamics) Consider a spherical particle moving in a fluid, such as water, with position  $x \in \mathbb{R}^d$ . Suppose the particle feels potential energy  $U(x)$ , which could come for example from gravity, from electrostatic interactions if the particle has a charge, etc. For a micron-scale particle (radius  $R \sim 1\mu\text{m}$ ), it is intractable to model all the degrees of freedom of the solvent, and a good model for the particle's dynamics is the *overdamped Langevin equation* (also called *Brownian dynamics*),

$$dX_t = -\frac{\nabla U(X_t)}{\gamma} dt + \sqrt{\frac{2k_B T}{\gamma}} dW_t, \quad X_t, W_t \in \mathbb{R}^d. \quad (34)$$

The first term on the RHS captures the force the particle feels due to the potential energy, where  $\gamma$  is the friction coefficient the particle feels due to the fluid; this is given by the Stokes-Einstein relation  $\gamma = 6\pi\eta R$  where  $\eta$  is the dynamic viscosity of the fluid. The second term captures the fluctuations the particle feels from the solvent, which is not a continuum at these scales, but rather fluctuates because it is made of a collection of discrete molecules. The remaining terms are the temperature  $T$  and Boltzmann's constant  $k_B$ . The corresponding Fokker-Planck equation is

$$\partial_t \rho = \nabla \cdot \left( \frac{1}{\gamma} \nabla U(x) \rho \right) + \frac{k_B T}{\gamma} \Delta \rho.$$

To find the stationary distribution, let's look for a solution with  $\underline{j} = 0$ :

$$\frac{1}{\gamma} \nabla U(x) \rho + \frac{k_B T}{\gamma} \nabla \rho = 0 \quad \Rightarrow \quad \frac{\nabla \rho}{\rho} = -(k_B T)^{-1} \nabla U \quad \Rightarrow \quad \ln \rho = -(k_B T)^{-1} U(x) + C.$$

The stationary distribution is therefore

$$\rho(x) = Z^{-1} e^{-U(x)/k_B T}, \quad Z = \int_{\mathbb{R}^d} e^{-U(x)/k_B T} dx,$$

provided  $Z < \infty$ . This is the *Boltzmann distribution*, or *Gibbs measure*. It is known to be the stationary distribution for a physical system in equilibrium, i.e. one with no external, non-conservative forces. This shows that (34) is a candidate for a model of the dynamics of a system whose stationary distribution is known to be the Boltzmann distribution.

**Example 10.8** Example 10.7 is also useful if we have a probability distribution  $\pi(x)$  and we wish to generate samples from this probability distribution. Defining  $U(x) = -\log \pi(x)$ , we have that  $\pi(x) = e^{-U(x)}$  so from our previous calculations, the stochastic process

$$dX_t = \nabla \log \pi(X_t) + \sqrt{2}dW_t$$

has the desired stationary distribution. Therefore, if we simulate the above process, we expect that after long times (given suitable ergodicity assumptions),  $X_t \sim \pi$ . This idea is useful in sampling high-dimensional probability distributions, such as likelihood functions that arise in Bayesian analysis; a particularly nice property is that  $\pi$  doesn't need to be normalized.

Notice that in all of these examples we looked for a solution with  $\underline{j} = 0$ . This is a much stronger condition than  $\nabla \cdot \underline{j} = 0$ , so we shouldn't always expect to find such a solution. However, if we do find a solution, then we are done, since (usually) the solution is unique. We will see in a future lecture that we can tell, from the coefficients of the SDE, when a solution satisfying the stronger condition  $\underline{j} = 0$  will be possible. Such systems with no steady-state flux, will correspond to "equilibrium" or reversible systems, which satisfy detailed balance.

**Example 10.9** (Sticky Brownian Motion) Consider a Brownian motion on  $[0, 1]$ , which can "stick" (spend finite time at) a boundary at  $x = 0$ , and which reflects off a boundary at  $x = 1$ . The forward equation is

$$\frac{1}{2}\Delta f = 0, \quad f_x = \kappa f_{xx}|_{x=0}, \quad f_x = 0|_{x=1}.$$

Notice the unusual boundary condition at  $x = 0$ . Let's show the stationary distribution is  $\rho(x) = \frac{1}{1+\kappa}(1 + \kappa\delta(x))$ . Notice that we can't compute  $\mathcal{L}^*\rho$  directly, since  $\rho$  contains a delta-function (even defining  $\mathcal{L}^*$  is tricky). Therefore we must use the weak formulation of the FP equation, and show that  $\langle \mathcal{L}f, \rho \rangle = 0$  for all test functions  $f$ . We compute (leaving out the normalization factor):

$$\begin{aligned} \langle \mathcal{L}f, \rho \rangle &= \int f_{xx}(1 + \kappa\delta(x))dx \\ &= f_x|_0^1 + \kappa f_{xx}(0) \\ &= 0 - f_x(0) + \kappa f_{xx}(0) && \text{(boundary condition at 1)} \\ &= 0. && \text{(boundary condition at 0)} \end{aligned}$$

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