Forward Master equation and forward Kolmogorov equation (Fokker-Planck) equation

1 Heuristics for diffusion processes

Let us, as usual, denote by $\boldsymbol{\phi}_t$ the diffusion process describing fundamental solution of the Ito stochastic differential equation

$$d\boldsymbol{\xi}_t = \boldsymbol{b}\,(\boldsymbol{\xi}_t, t)\ dt + \mathsf{A}(\boldsymbol{\xi}_t, t) \cdot d\boldsymbol{\omega}_t \tag{1.1}$$

As before we define the diffusivity matrix as $\mathsf{G} := \mathsf{A}\mathsf{A}^{\dagger}$ For any given initial condition $\boldsymbol{x}_o$ at time t_o we have for $t \geq 0$

$$\mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) = \mathrm{E}\, \delta^{(d)}(\boldsymbol{x} - \boldsymbol{\phi}_t(t_o, \boldsymbol{x}_o))$$

Differentiating both sides with respect to time applying Ito lemma and the martingale property of stochastic increments we get into

$$\partial_t \mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) = \partial_t \mathrm{E}\, \delta^{(d)}(\boldsymbol{x} - \boldsymbol{\phi}_t(t_o, \boldsymbol{x}_o))$$
$$\mathrm{E}\left\{ \left[\boldsymbol{b}\,(\boldsymbol{\phi}_t, t) \cdot \partial_{\boldsymbol{\phi}_t} + \frac{1}{2} \mathsf{G}\,(\boldsymbol{\phi}_t, t) : \partial_{\boldsymbol{\phi}_t} \partial_{\boldsymbol{\phi}_t} \right] \delta^{(d)}(\boldsymbol{x} - \boldsymbol{\phi}_t(t_o, \boldsymbol{x}_o)) \right\}$$

Using the translational invariance of the δ-function we can write the right hand side as

$$\partial_t \mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) =$$
$$\mathrm{E}\left\{ \left[-\boldsymbol{b}\,(\boldsymbol{\phi}_t, t) \cdot \partial_{\boldsymbol{x}} + \frac{1}{2} \mathsf{G}\,(\boldsymbol{\phi}_t, t) : \partial_{\boldsymbol{x}} \partial_{\boldsymbol{x}} \right] \delta^{(d)}(\boldsymbol{x} - \boldsymbol{\phi}_t(t_o, \boldsymbol{x}_o)) \right\}$$

and then carry the derivatives over the average sign

$$\partial_t \mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) =$$
$$-\partial_{\boldsymbol{x}} \cdot \mathrm{E}\, \boldsymbol{b}\,(\boldsymbol{\phi}_t, t)\, \delta^{(d)}(\boldsymbol{x} - \boldsymbol{\phi}_t(t_o, \boldsymbol{x}_o)) + \partial_{\boldsymbol{x}} \partial_{\boldsymbol{x}} : \mathrm{E}\, \frac{\mathsf{G}\,(\boldsymbol{\phi}_t, t)}{2} \delta^{(d)}(\boldsymbol{x} - \boldsymbol{\phi}_t(t_o, \boldsymbol{x}_o))$$

From the properties of the δ-function we finally conclude

$$\partial_t \mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) = \partial_{\boldsymbol{x}} \cdot \boldsymbol{J}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) \tag{1.2a}$$

$$\boldsymbol{J}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) = -\boldsymbol{b}\,(\boldsymbol{x}, t)\, \mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) + \partial_{\boldsymbol{x}} \cdot \left[\frac{\mathsf{G}\,(\boldsymbol{x}, t)}{2} \mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) \right] \tag{1.2b}$$

We thus derived the Fokker-Planck equation:

$$\partial_t \mathrm{p}_{\boldsymbol{\xi}} = -\partial_{\boldsymbol{x}} \cdot (\boldsymbol{b}\, \mathrm{p}_{\boldsymbol{\xi}}) + \frac{1}{2} \partial_{\boldsymbol{x}} \partial_{\boldsymbol{x}} : (\mathsf{G}\, \mathrm{p}_{\boldsymbol{\xi}}) \tag{1.3}$$

In the probabilistic literature (1.2a) or equivalently (1.3) are referred to as *forward Kolmogorov* equation. The describe the forward in time t evolution of a transition probability density satisfying under our hypothesis the *initial condition*

$$\lim_{t \to t_o} \mathrm{p}_{\boldsymbol{\xi}}(\boldsymbol{x}, t, \,|\, \boldsymbol{x}_o, t_o) = \delta^{(d)}(\boldsymbol{x} - \boldsymbol{x}_o) \tag{1.4}$$

2 Master equation for Markov processes with jumps

Proposition 2.1. *Let us suppose that the* $\mathbb{S}$*-valued Markov process* $\boldsymbol{\xi}_t$ *satisfies for* $t \in [t_{\mathrm{o}}, t_{\mathrm{f}}]$ *the hypotheses* i *(jump condition),* ii *(drift condition),* iii *(diffusivity condition) of* lecture 14. *Then as function of the conditioned event the transition probability density of the Markov process satisfies the integro-differential equation*

$$(\partial_t - \mathfrak{L}^{\dagger}_{\boldsymbol{x}})\mathrm{p}(\boldsymbol{x}, t|\cdot) = \fint_{\mathbb{S}} d^d z \, [\mathrm{K}_t(\boldsymbol{x}|\boldsymbol{z})\mathrm{p}(\boldsymbol{z}, t|\cdot) - \mathrm{K}_t(\boldsymbol{z}|\boldsymbol{x})\mathrm{p}(\boldsymbol{x}, t|\cdot)] \tag{2.1}$$

where $\fint_{\mathbb{S}}$ *is the principal value integral and* $\mathfrak{L}$ *is the adjoint of the continuous part of the generator of the process.*

Proof. Let f be an arbitrary, smooth and integrable test function. The we have

$$\begin{aligned} \partial_t \mathrm{E}_{\bullet} f(\boldsymbol{\xi}_t) &= \partial_t \int_{\mathbb{S}} d^d x \, f(\boldsymbol{x}) \, \mathrm{p}(\boldsymbol{x}, t \,|\, \cdot) \\ &= \lim_{dt \downarrow 0} \int_{\mathbb{S}^2} d^d x \, d^d z \, \frac{f(\boldsymbol{x}) - f(\boldsymbol{z})}{dt} \mathrm{p}(\boldsymbol{x}, t + dt \,|\, \boldsymbol{z}\,, t) \, \mathrm{p}(\boldsymbol{z}, t \,|\, \cdot) \end{aligned} \tag{2.2}$$

For arbitrary ε we can define

$$V^{\varepsilon}_{\boldsymbol{z}} := \{\boldsymbol{x} \in \mathbb{S} \,|\, \parallel \boldsymbol{x} - \boldsymbol{z} \parallel \leq \varepsilon\} \tag{2.3}$$

and $\bar{V}^{\varepsilon}_{\boldsymbol{z}} := \mathbb{S}/V^{\varepsilon}_{\boldsymbol{z}}$. We have on the one hand

$$\begin{aligned} &\int_{V^{\varepsilon}_{\boldsymbol{z}}} d^d x \, \frac{f(\boldsymbol{x}) - f(\boldsymbol{z})}{dt} \mathrm{p}(\boldsymbol{x}, t + dt \,|\, \boldsymbol{z}\,, t) \\ &= \int_{V^{\varepsilon}_{\boldsymbol{z}}} d^d x \, \left[\frac{(\boldsymbol{x} - \boldsymbol{z}) \cdot \partial_{\boldsymbol{z}} + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{z}) \otimes (\boldsymbol{x} - \boldsymbol{z}) : \partial_{\boldsymbol{z}} \otimes \partial_{\boldsymbol{z}}}{dt} f(\boldsymbol{z}) + o(\parallel \boldsymbol{x} - \boldsymbol{z} \parallel^2) \right] \mathrm{p}(\boldsymbol{x}, t + dt \,|\, \boldsymbol{z}\,, t) \end{aligned} \tag{2.4}$$

Taking the first the limit $dt \downarrow 0$ and then $\varepsilon \downarrow 0$ since the drift and diffusivity conditions hold for arbitrary ε we obtain

$$\lim_{\varepsilon \downarrow 0} \partial_t \mathrm{E}_{\bullet} f(\boldsymbol{\xi}_t) \mathbb{1}_{V^{\varepsilon}_{\boldsymbol{z}}} = \int_{\mathbb{S}} d^d x \, (\mathfrak{L}_{\boldsymbol{x}} f)(\boldsymbol{x}, t) \, \mathrm{p}(\boldsymbol{x}, t \,|\, \cdot) \tag{2.5}$$

On the other hand, we have by the jump-rate condition i

$$\begin{aligned} &\lim_{dt \downarrow 0} \int_{\bar{V}^{\varepsilon}_{\boldsymbol{z}} \times \mathbb{S}} d^d x \, d^d z \, \frac{f(\boldsymbol{x}) - f(\boldsymbol{z})}{dt} \mathrm{p}(\boldsymbol{x}, t + dt \,|\, \boldsymbol{z}\,, t) \, \mathrm{p}(\boldsymbol{z}, t \,|\, \cdot) \\ &\quad = \int_{\bar{V}^{\varepsilon}_{\boldsymbol{z}} \times \mathbb{S}} d^d x \, d^d z \, [f(\boldsymbol{x}) - f(\boldsymbol{z})] \, \mathrm{K}_t(\boldsymbol{x} \,|\, \boldsymbol{z}) \, \mathrm{p}(\boldsymbol{z}, t \,|\, \cdot) = \partial_t \mathrm{E}_{\bullet} f(\boldsymbol{\xi}_t) \mathbb{1}_{\bar{V}^{\varepsilon}_{\boldsymbol{z}}} \end{aligned} \tag{2.6}$$

Gathering the two contributions we obtain

$$\int_{\mathbb{S}} d^d x \, f(\boldsymbol{x}) \left\{ (\partial_t - \mathfrak{L}^{\dagger}_{\boldsymbol{x}}) \mathrm{p}(\boldsymbol{x}, t \,|\, \cdot) - \fint_{\mathbb{S}} d^d z \, [\mathrm{K}_t(\boldsymbol{x} \,|\, \boldsymbol{z}) \, \mathrm{p}(\boldsymbol{z}, t \,|\, \cdot) - \mathrm{K}_t(\boldsymbol{z} \,|\, \boldsymbol{x}) \, \mathrm{p}(\boldsymbol{x}, t \,|\, \cdot)] \right\} = 0 \tag{2.7}$$

where in general

$$\begin{aligned} &\int_{\mathbb{S}} d^d x \, f(\boldsymbol{x}) \, \mathfrak{L}^{\dagger}_{\boldsymbol{x}} \mathrm{p}(\boldsymbol{x}, t \,|\, \cdot) = \\ &\quad - \int_{\partial \mathbb{S}} d^{d-1} x \, [f(\boldsymbol{x}) \, \boldsymbol{n} \cdot \boldsymbol{J}(\boldsymbol{x}, t|\cdot) + \mathrm{p}(\boldsymbol{x}, t|\cdot) \boldsymbol{n} \cdot \partial_{\boldsymbol{x}} f(\boldsymbol{x})] + \int_{\mathbb{S}} d^d x \, f(\boldsymbol{x}) \partial_{\boldsymbol{x}} \cdot \boldsymbol{J}(\boldsymbol{x}, t|\cdot) \end{aligned} \tag{2.8a}$$

$$\boldsymbol{J}(\boldsymbol{x}, t|\cdot) := -\boldsymbol{b}(\boldsymbol{x}, t) \, \mathrm{p}(\boldsymbol{x}, t|\cdot) + \frac{1}{2} \partial_{\boldsymbol{x}} \cdot \mathsf{G}(\boldsymbol{x}, t) \, \mathrm{p}(\boldsymbol{x}, t|\cdot) \tag{2.8b}$$

for $\boldsymbol{n}$ the unit vector orthogonal and outwards pointing to $\partial \mathbb{S}$. The arbitrariness of f implies that the (2.7) vanishes generically only if the argument of the curly brackets vanishes, as claimed. □

3 Forward Kolmogorov equation (Fokker-Planck) equation

The adjoint $\mathfrak{L}^{\dagger}$ reduces to the differential operation

$$\mathfrak{L}^{\dagger} = -\boldsymbol{b}(\boldsymbol{x}, t) \cdot \partial_{\boldsymbol{x}} + \partial_{\boldsymbol{x}} \otimes \partial_{\boldsymbol{x}} : \mathsf{G}(\boldsymbol{x}, t) \tag{3.1}$$

if

$$f(\boldsymbol{x})\, \boldsymbol{n} \cdot \boldsymbol{J}(\boldsymbol{x}, t|\cdot) + \mathrm{p}(\boldsymbol{x}, t|\cdot) \boldsymbol{n} \cdot \partial_{\boldsymbol{x}} f(\boldsymbol{x}) = 0 \tag{3.2}$$

for all $\boldsymbol{x} \in \partial\mathbb{S}$. There are at least four interesting cases when this circumstance occurs.

- Probability conservation:

$$\boldsymbol{n} \cdot \boldsymbol{J}(\boldsymbol{x}, t|\cdot) = 0 \qquad \forall\, \boldsymbol{x} \,\in\, \partial\mathbb{S} \tag{3.3}$$

  The geometric interpretation of this condition is intuitive. The vanishing of the probability current on the boundary of the domain $\mathbb{S}$ should enforce probability conservation: if we formally write the current as the sum

$$\boldsymbol{J} = \boldsymbol{J}_{\mathrm{outwards}} + \boldsymbol{J}_{\mathrm{inwards}} \qquad \text{such that} \qquad \begin{aligned} \boldsymbol{n} \cdot \boldsymbol{J}_{\mathrm{outwards}}|_{\mathbb{S}} &\geq 0 \\ \boldsymbol{n} \cdot \boldsymbol{J}_{\mathrm{inwards}}|_{\mathbb{S}} &< 0 \end{aligned}$$

  we can interpret (3.3) as a *reflecting boundary* condition: all incoming trajectories from the interior of $\mathbb{A}_d$ to the boundary $\partial\mathbb{S}$ are subsequently reflected to the interior of $\mathbb{S}$.

  In order (3.9) the condition must be accompanied by

$$\boldsymbol{n} \cdot \partial_{\boldsymbol{x}} f(\boldsymbol{x}) = 0 \qquad \forall\, \boldsymbol{x} \,\in\, \partial\mathbb{S} \tag{3.4}$$

  This second condition in the proof of the proposition above appears as constraint on the admissible test functions f. This is also a constraint on the functional space dual to the transition probability density of the Markov process. More explicitly the Chapman-Kolmogorov equation for any $t_2 \,\geq\, t_1$

$$\mathrm{p}(\boldsymbol{x}_2, t_2 \,|\, \boldsymbol{x}_1, t_1) = \int_{\mathbb{S}} d^d x\, \mathrm{p}(\boldsymbol{x}_2, t_2 \,|\, \boldsymbol{x}, t)\, \mathrm{p}(\boldsymbol{x}, t \,|\, \boldsymbol{x}_1, t_1) \tag{3.5}$$

  requires

$$0 = \partial_t \mathrm{p}(\boldsymbol{x}_2, t_2 \,|\, \boldsymbol{x}_1, t_1) = -\int_{\mathbb{S}} d^d x\, [(\mathfrak{L}_{\boldsymbol{x}} \mathrm{p})(\boldsymbol{x}_2, t_2 \,|\, \boldsymbol{x}, t)\, \mathrm{p}(\boldsymbol{x}, t \,|\, \boldsymbol{x}_1, t_1) + \mathrm{p}(\boldsymbol{x}_2, t_2 \,|\, \boldsymbol{x}, t)\, \partial_t \mathrm{p}(\boldsymbol{x}, t \,|\, \boldsymbol{x}_1, t_1)] \tag{3.6}$$

  Combining this latter equation with (3.1) and (3.3) imposes that

$$\boldsymbol{n} \cdot \partial_{\boldsymbol{x}} \mathrm{p}(\cdot \,|\, \boldsymbol{x}, t) = 0 \qquad \forall\, \boldsymbol{x} \in \partial\mathbb{S} \tag{3.7}$$

  is the boundary condition satisfied by the backward Kolmogorov equation if probability is to be conserved in $\mathbb{S}$.

- Probability absorption:

$$p(\boldsymbol{x}, t|\cdot) = 0 \qquad \forall\, \boldsymbol{x} \in \partial\mathbb{S} \tag{3.8}$$

  By (3.6) this condition entails

$$f(\boldsymbol{x}) = p(\cdot|\boldsymbol{x}, t) = 0 \qquad \forall\, \boldsymbol{x} \in \partial\mathbb{S} \tag{3.9}$$

  for elements on the dual space.

- $\mathbb{S}$ unbounded (e.g. $\mathbb{S} = \mathbb{R}^d$): integrability requires (3.3) and (3.8) to coincide
- $\mathbb{S} = \mathbb{T}^d$: periodic boundary conditions.