Outline

1. Setting
2. Bayes rule and the Brownian score
   - Looking backward
   - The Brownian computation
   - Example: two clusters
3. The Kolmogorov route
   - Reversed transition density
   - Anderson's computation
   - The time reversal theorem
4. The variance preserving equation

Conditional densities Consider a couple (X, Z) or r.v. with $X, Z \in \mathbb{R}^n$. Assume that (X, Z) has a joint density

$$f(x, z), \quad x, z \in \mathbb{R}^n$$

such that $A \subset \mathbb{R}^n \times \mathbb{R}^n$

$$\mathbb{P}((X, Z) \in A) = \int_A f(x, z)\, dx\, dz$$

$$\mathbb{E}[g(X, Z)] = \int_{\mathbb{R}^n \times \mathbb{R}^n} f(x, z)\, g(x, z)\, dx\, dz$$

Formula for cond. density

$$f_{Z|X}(z|x) = \frac{f(x,z)}{f_X(x)}$$

where the marginal density is

$$f_X(x) = \int_{\mathbb{R}^n} f(x,z)\, dz$$

Rmk Once we have the cond. density

$$\mathbb{E}[\varphi(Z)|X=x] = \int_{\mathbb{R}^n} \varphi(z) f_{Z|X}(z|x)\, dz$$

$$\mathbb{E}[\varphi(Z)|X] = \int_{\mathbb{R}^n} \varphi(z) f_{Z|X}(z|x)\, dz \,\Big|_{x=X}$$

Rmk Our aim is to identify the coefficient of the diffusion

$$\hat{X}_t \equiv X_{T-t}$$

by 2 means

Focus today, with X = Wiener process

(1) **Drift**

$$= \lim_{h \to \infty} \frac{1}{h} \mathbb{E}\left[\left(\hat{X}_{s+h} - x \right) \mid X_s = x \right]$$

Diffusion coefficient → conditional variance

(2) Kolmogorov equations → $\hat{\mathcal{L}}_s$ → read coeff

First step: Conditional density of X_{s-h} given $X_s = x$

Our vector is (X_s, X_{s-h}) — X_s: x, X_{s-h}: z

Joint density: (Markov)

$$f(x, z) = p_{s-h}(z)\, \tilde{q}_{s-h,s}(z, x)$$

$p_{s-h}(z)$: Density at time $s-h$

$\tilde{q}_{s-h,s}(z, x)$: Transition $s-h \to s$

Cond. density

$$f_{X_{s-h} | X_s}(z \mid x) = \frac{p_{s-h}(z)\, \tilde{q}_{s-h,s}(z, x)}{p_s(x)}$$

Conditional mean

density of X_{s-h} when Brownian dynamics

cond. density

$$\frac{1}{h}\mathbb{E}\left[X_{s-h} - x \mid X_s = x \right] = \frac{1}{h} \int_{\mathbb{R}^n} (z-x) \frac{p_{s-h}(z)\, \tilde{q}_{s-h,s}(z,x)}{p_s(x)}\, dz$$

Brownian case

Gaussian kernel

$$\tilde{q}_{s-h,s}(z,x) = g_h(z-x) = \frac{1}{(2\pi h)^{n/2}} \exp\left(-\frac{|z-x|^2}{2h} \right)$$

$$p_s(x) = \int \mu(dz)\, \tilde{q}_{0,s}(z,x)$$

non Gaussian!

$$\frac{1}{h}\mathbb{E}\left[X_{s-h}-x \mid X_s = x\right]$$

$$= \frac{1}{h}\int_{\mathbb{R}^n} (z-x)\, \frac{p_{s-h}(z)\, \tilde{q}_{s-h,s}(z,x)}{p_s(x)}\, dz$$

$$\tilde{q}_{s-h,s}(z,x) = \frac{1}{(2\pi h)^{n/2}} \exp\left(-\frac{|z-x|^2}{2h}\right)$$

Natural cv: $\frac{z-x}{\sqrt{h}} = \xi$. Then

$$\tilde{q}_{s-h,s}(z,x) = \frac{1}{h^{n/2}}\, \phi(\xi) = \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{|\xi|^2}{2}\right)$$

↳ density of $\mathcal{N}(0, \mathrm{Id})$

$$dz = h^{n/2}\, d\xi \quad , \quad z - x = \sqrt{h}\,\xi$$

$$\Rightarrow \boxed{\frac{1}{h}\mathbb{E}\left[X_{s-h} - x \mid X_s = x\right] \quad \frac{1}{\sqrt{h}} \int_{\mathbb{R}^n} \xi\, \frac{p_{s-h}(x+\sqrt{h}\,\xi)\, \phi(\xi)}{p_s(x)}\, d\xi}$$

$$\frac{1}{h}\mathbb{E}\left[X_{s-h}-x \mid X_s=x\right] = \frac{1}{\sqrt{h}}\int_{\mathbb{R}^n} \xi \, \frac{p_{s-h}(x+\sqrt{h}\xi)\,\phi(\xi)}{p_s(x)}\, d\xi$$

Taylor in h:

$$p_{s-h}(x+\sqrt{h}\xi) = p_s(x) + \sqrt{h}\,\xi^T \nabla p_s(x) + O(h)$$

$$\Rightarrow \frac{1}{h}\mathbb{E}\left[X_{s-h}-x \mid X_s=x\right]$$

$$= \int_{\mathbb{R}^n} \frac{d\xi}{\sqrt{h}}\,\phi(\xi)\,\xi \left\{ \frac{p_s(x) + \sqrt{h}\,\xi^T \nabla p_s(x) + O(h)}{p_s(x)} \right\}$$

$$= \underbrace{\mathbb{E}\left[\mathcal{N}(0, Id)\right] = 0}$$

$$= \frac{1}{\sqrt{h}} \int_{\mathbb{R}^n} \xi\,\phi(\xi)\,d\xi + \Big(\underbrace{\int_{\mathbb{R}^n} \xi\,\xi^T \phi(\xi)\,d\xi}_{= Id_{\mathbb{R}^n}} \Big) \frac{\nabla p_s(x)}{p_s(x)}$$

$$+ O(\sqrt{h})$$

$$= \frac{\nabla p_s(x)}{p_s(x)} + O(\sqrt{h}) = \nabla(\log p_s(x)) + O(\sqrt{h})$$

Conclusion

$$\lim_{h \to 0} \frac{1}{h} \mathbb{E}\left[(X_{s-h} - x) \mid X_s = x \right]$$

$$= \nabla (\log p_s(x)) = \frac{\nabla p_s(x)}{p_s(x)}$$

$\Rightarrow$ Drift of reversed dynamics is

$\nabla (\log p_{T-t}(\hat{X}_t))$ $\equiv$ score function

Rmk: X had no drift

$\hat{X}$ gets a drift (score func.)

($\simeq$ gradient descent where $\hat{X}$ is likely)

Rmk : In the same way, when X is $X_0 + W$, the diffusion coefficient of $\hat{X}$ is identified as Id

$\Rightarrow$ If $X_t = X_0 + W_t$, then

$\hat{X}_t \equiv X_{T-t}$ satisfies

$$d\hat{X}_t = \nabla \log p_{T-t}(\hat{X}_t)\, dt + d\hat{W}_t$$

Conditional densities (recall)

Setting: Couple (X, Z) in $\mathbb{R}^n \times \mathbb{R}^n$

- With joint density $f(x, z)$
- Marginal density of X: $f_X(x) = \int_{\mathbb{R}^n} f(x, z)\, dz$

Bayes rule: For x such that $f_X(x) > 0$
$\hookrightarrow$ conditional density of Z given $X = x$

$$f_{Z|X}(z \,|\, x) = \frac{f(x, z)}{f_X(x)}$$

Conditional expectation: For φ bounded measurable,

$$\mathbf{E}\left[\varphi(Z) \,|\, X = x\right] = \frac{1}{f_X(x)} \int_{\mathbb{R}^n} \varphi(z)\, f(x, z)\, dz$$

Looking backward: Bayes rule

Joint density: For $0 < s - h < s$, by the Markov property

$$(X_{s-h}, X_s) \text{ has density } (z, x) \mapsto p_{s-h}(z)\, \widetilde{q}_{s-h,s}(z, x)$$

Bayes rule: With $X = X_s$ and $Z = X_{s-h}$, we get

$$f_{X_{s-h}|X_s}(z \,|\, x) = \frac{p_{s-h}(z)\, \widetilde{q}_{s-h,s}(z, x)}{p_s(x)}$$

Reading:

- Forward transition $\widetilde{q}_{s-h,s}(\cdot, x)$, reweighted by p_{s-h}
- Transition of $\widehat{X}$, explicit in terms of p and $\widetilde{q}$

Reading coefficients from moments (recall)

Infinitesimal drift and covariance: For the forward diffusion,

$$\lim_{h \to 0^+} \frac{1}{h} \mathbf{E}\left[X_{s+h} - X_s \,|\, \mathcal{F}_s\right] = b(s, X_s)$$
$$\lim_{h \to 0^+} \frac{1}{h} \mathbf{Cov}\left(X_{s+h} - X_s \,|\, \mathcal{F}_s\right) = a(s)$$

Strategy for the time reversal equation: Take backward limits

- Backward mean: $\lim_{h \to 0^+} \frac{1}{h} \mathbf{E}\left[X_{s-h} - X_s \,|\, X_s = x\right]$
- Backward second moment: $\lim_{h \to 0^+} \frac{1}{h} \mathbf{E}\left[(X_{s-h} - X_s)^{\otimes 2} \,|\, X_s = x\right]$
- These limits: drift and diffusion matrix of $\widehat{X}$, if it is a diffusion

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Brownian case

Setting: $b \equiv 0$ and $\sigma \equiv \mathrm{Id}$, that is $X = X_0 + W$ with $X_0 \sim \mu$

Heat kernel: Transition density

$$\begin{aligned} \widetilde{q}_{s,t}(x,y) &= g_{t-s}(y-x) \\ g_u(w) &= \frac{1}{(2\pi u)^{n/2}} \exp\left(-\frac{|w|^2}{2u}\right) \end{aligned}$$

Marginal density:

$$p_s(x) = \int_{\mathbb{R}^n} g_s(x-z)\,\mu(dz) = (\mu * g_s)(x)$$

$\hookrightarrow$ Smooth and positive for $s > 0$, whatever μ

Backward drift of Brownian motion

Proposition 1

Consider:

- $X = X_0 + W$ *with* $X_0 \sim \mu$
- $p_s = \mu * g_s$ *the density of* X_s

Then for $s \in (0, \tau]$ *and* $x \in \mathbb{R}^n$*, we have*

$$\lim_{h \to 0^+} \frac{1}{h} \mathbf{E}\left[X_{s-h} - X_s \,|\, X_s = x\right] = \nabla \log p_s(x)$$

Remark: Forward, Brownian motion has no drift

$\hookrightarrow$ Backward, it acquires the drift $\nabla \log p_s$

Proof sketch for Proposition 1 (1)

Formal computation: Taylor expansions, limits under the integral sign

Bayes rule: Conditional density of X_{s-h} given $X_s = x$
$\hookrightarrow$ with $\widetilde{q}_{s-h,s}(z, x) = g_h(x - z)$

$$\frac{1}{h}\,\mathbf{E}\left[X_{s-h} - X_s \,|\, X_s = x\right] = \frac{1}{h}\int_{\mathbb{R}^n} (z - x)\,\frac{p_{s-h}(z)\,g_h(x - z)}{p_s(x)}\,dz$$

Proof sketch for Proposition 1 (2)

Gaussian scaling:

- Change of variables $z = x + \sqrt{h}\,\xi$
  $\hookrightarrow$ so that $dz = h^{n/2}\,d\xi$ and $z - x = \sqrt{h}\,\xi$
- Scaling: $h^{n/2} g_h(\sqrt{h}\,\xi) = \phi(\xi)$, standard Gaussian density
- g_h even, hence $g_h(x - z)\,dz = \phi(\xi)\,d\xi$

Then we have:

$$\frac{1}{h}\,\mathbf{E}\left[X_{s-h} - X_s \,|\, X_s = x\right] = \frac{1}{\sqrt{h}} \int_{\mathbb{R}^n} \xi\, \frac{p_{s-h}(x + \sqrt{h}\,\xi)}{p_s(x)}\, \phi(\xi)\,d\xi$$

$\hookrightarrow$ Prefactor $h^{-1/2}$ diverges: a cancellation is needed

Proof sketch for Proposition 1 (3)

Taylor expansion of the tilt: Around (s, x),

$$\frac{p_{s-h}(x + \sqrt{h}\,\xi)}{p_s(x)} = 1 + \sqrt{h}\,\xi \cdot \nabla \log p_s(x) + O(h)$$

Plugging into the previous slide: Formally,

$$\frac{1}{h}\,\mathbf{E}\left[X_{s-h} - X_s \,|\, X_s = x\right]$$
$$= \frac{1}{\sqrt{h}} \int_{\mathbb{R}^n} \xi\,\phi(\xi)\,d\xi + \int_{\mathbb{R}^n} \xi\,(\xi \cdot \nabla \log p_s(x))\,\phi(\xi)\,d\xi + O(\sqrt{h})$$

Proof sketch for Proposition 1 (4)

Three contributions:

- Order $h^{-1/2}$: vanishes, since $\int \xi \, \phi(\xi) \, d\xi = 0$
- Order 1: survives, since $\int \xi \xi^* \, \phi(\xi) \, d\xi = \mathrm{Id}$
- Order $\sqrt{h}$: vanishes in the limit

Conclusion: Only the order 1 term survives

$$\lim_{h \to 0^+} \frac{1}{h} \mathbf{E} \left[X_{s-h} - X_s \,|\, X_s = x \right] = \mathrm{Id} \, \nabla \log p_s(x) = \nabla \log p_s(x)$$

Backward covariance

Proposition 2

Let $\Delta_h = X_{s-h} - X_s$. *For* $s \in (0, \tau]$ *and* $x \in \mathbb{R}^n$,

$$\lim_{h \to 0^+} \frac{1}{h} \mathbf{E}\left[\Delta_h^i \Delta_h^j \,|\, X_s = x\right] = \delta_{ij}$$

Formal proof: Same Bayes rule and same scaling

- Quadratic integrand: $(z-x)^i(z-x)^j = h\,\xi_i\xi_j$ absorbs h^{-1}
- Leading term 1 of the tilt: $\int \xi_i\xi_j\,\phi(\xi)\,d\xi = \delta_{ij}$
- Other terms of order $\sqrt{h}$: vanish

Reading the computation

Where the drift comes from:

- Gaussian $g_h(x - \cdot)$: past positions symmetric around x
- Tilt by p_{s-h}: more likely origins are preferred
- Tilt of order $\sqrt{h} \times$ displacement of order $\sqrt{h} =$ drift of order h

Direction: $\nabla \log p_s = \nabla p_s / p_s$
$\hookrightarrow$ Steepest relative increase of the density of X_s

Diffusion matrix unchanged: Even (second-order) quantity
$\hookrightarrow$ Blind to the direction of time

Identifying coefficients in reversed time

Reversed clock:

- Time t for $\widehat{X}$ is time $\tau - t$ for X
- Drift of $\widehat{X}$ at time t: $\nabla \log p_{\tau - t}$. Diffusion matrix: Id

Guess:

$$d\widehat{X}_t = \nabla \log p_{\tau - t}(\widehat{X}_t)\, dt + d\widehat{W}_t$$

Comments:

- Forward: no drift. Backward: time dependent drift
- $\widehat{X}$ drifts toward regions where $X_{\tau - t}$ is likely

The score

Definition 3

Let p_s be a positive $\mathcal{C}^1$ density on $\mathbb{R}^n$. The score of p_s is

$$x \longmapsto \nabla \log p_s(x) = \frac{\nabla p_s(x)}{p_s(x)}$$

Properties:

- Insensitive to normalization: $\nabla \log(c\, p_s) = \nabla \log p_s$
- Depends on μ through the whole evolution
- Only unknown term of the reversed drift: learned in Chapter 6