11/20 # Lecture 22: Diffusion Models

① $\boxed{\text{Fokker-Planck equations for forward + reverse processes are time reversals of each other.}}$

Forward: $dx_t = -x_t\,dt + \sqrt{2}\,dB_t$

$$\partial_t q_t = -\mathrm{div}\left(-x \cdot q_t\right) + \Delta q_t = \mathrm{div}(x \cdot q_t) + \Delta q_t$$

Reverse: $dx_t^{\leftarrow} = \left(x_t^{\leftarrow} + 2\nabla \ln q_{T-t}(x_t^{\leftarrow})\right) dt + \sqrt{2}\,dB_t$

$$\partial_t q_t^{\leftarrow} = -\mathrm{div}\left(\left(x + 2\nabla \ln q_t^{\leftarrow}\right) \cdot q_t^{\leftarrow}\right) + \Delta q_t^{\leftarrow}$$

Note $\mathrm{div}\left(\left(\nabla \ln q_t^{\leftarrow}\right) \cdot q_t^{\leftarrow}\right)$

$$= \mathrm{div}\left(\frac{\nabla q_t^{\leftarrow}}{q_t^{\leftarrow}} \cdot q_t^{\leftarrow}\right)$$

$$= \mathrm{div}\left(\nabla q_t^{\leftarrow}\right) = \Delta q_t^{\leftarrow}$$

$$= -\mathrm{div}(x \cdot q_t^{\leftarrow}) - \Delta q_t^{\leftarrow}$$

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② $\boxed{\text{Heuristic proof of Girsanov's:}}$

Given Ⓐ $dx_t = b_t\,dt + \sqrt{2}\,dB_t$

Ⓑ $dx_t = b_t'\,dt + \sqrt{2}\,dB_t$

Consider discrete-time approx, i.e.

$$\hat{x}_{(k+1)h} \leftarrow \hat{x}_{kh} + h \cdot b_{kh}(\hat{x}_{kh}) + \sqrt{2h}\, g_{kh}$$

$$\hat{x}_{(k+1)h} \leftarrow \hat{x}_{kh} + h \cdot b'_{kh}(\hat{x}_{kh}) + \sqrt{2h}\, g_{kh}$$

for $g_{kh} \sim N(0, I_d)$

Likelihood of observing trajectory

$$(\hat{x}_0, \hat{x}_h, \hat{x}_{2h}, \dots, \hat{x}_{Nh})$$

under (A) vs (B):

$$(A): \prod_{k=0}^{N-1} \exp\left(-\frac{1}{4h} \left\| \hat{x}_{(k+1)h} - \hat{x}_{kh} - h \cdot b_{kh}(\hat{x}_{kh}) \right\|^2\right)$$

$$(B): \prod_{k=0}^{N-1} \exp\left(-\frac{1}{4h} \left\| \hat{x}_{(k+1)h} - \hat{x}_{kh} - h \cdot b'_{kh}(\hat{x}_{kh}) \right\|^2\right)$$

$$\frac{(A)}{(B)} = \prod_{k=0}^{N-1} \exp\left(-\frac{1}{4h}\left[\|b_{kh}(\hat{x}_{kh})\|^2 \cdot h^2 - \|b'_{kh}(x_{kh})\|^2 \cdot h^2 - 2h \langle \underbrace{\hat{x}_{(k+1)h} - \hat{x}_{kh}}_{\substack{\text{under (B),} \\ \text{this } = h \cdot b'_{kh}(\hat{x}_{kh}) + \sqrt{2h}\, g_{kh}}}, b_{kh}(\hat{x}_{kh}) - b'_{kh}(\hat{x}_{kh}) \rangle \right]\right)$$

$$= \prod_{k=0}^{N-1} \exp\left(-\frac{1}{4h}\left[-\|b_{kh}(\hat{x}_{kh}) - b'_{kh}(\hat{x}_{kh})\|^2 \cdot h^2 \right.\right.$$

$$+ h \cdot 2\sqrt{2} \left\langle \sqrt{h}\, g_{kh},\ b_{kh}(\hat{x}_{kh}) - b'_{kh}(\hat{x}_{kh}) \right\rangle \Big)$$

$$= \exp\Bigg(-\frac{1}{4} \sum_{k=0}^{N-1} h \left\| b_{kh}(\hat{x}_{kh}) - b'_{kh}(\hat{x}_{kh}) \right\|^2 + \frac{1}{\sqrt{2}} \sum_{k=0}^{N-1} \Big\langle \underbrace{\sqrt{h}\, g_{kh}}_{\text{“} dB_{kh} \text{”}},\ b_{kh}(\hat{x}_{kh}) - b'_{kh}(\hat{x}_{kh}) \Big\rangle \Bigg)$$

$$\xrightarrow{(h \to 0)} \exp\left(-\frac{1}{4} \int_0^T \| b_t - b'_t \|^2 \, dt + \frac{1}{\sqrt{2}} \int_0^T \langle dB_t,\ b_t - b'_t \rangle \right)$$

So

$$KL(\text{Ⓐ} \,\|\, \text{Ⓑ}) =$$

$$\mathbb{E}_{\text{Ⓐ}} \left[-\frac{1}{4} \int_0^T \| b_t - b'_t \|^2 dt + \frac{1}{\sqrt{2}} \int_0^T \langle \underbrace{dB_t} ,\ b_t - b'_t \rangle \right] \quad (\star)$$

Brownian motion wrt. Ⓑ, so

$$\mathbb{E}_{\text{Ⓐ}}[\cdot] \neq 0\,!$$

Can also write dB_t in terms of Ⓐ by equating

$$b_t\,dt + \sqrt{2}\,d\hat{B}_t = b_t'\,dt + \sqrt{2}\,dB_t$$

$$\Rightarrow dB_t = \frac{1}{\sqrt{2}}\left(b_t - b_t'\right)dt + d\hat{B}_t .$$

Substituting into (✱) and noting $\mathbb{E}_{Ⓐ}\left[d\hat{B}_t\right] = 0$,

$$KL(Ⓐ \,\|\, Ⓑ) = \frac{1}{4}\mathbb{E}_{Ⓐ}\int_0^T \|b_t - b_t'\|^2\,dt \qquad \square$$

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③ Girsanov analysis for Langevin (will finish in next lecture)

ALG: $d\hat{x}_t = -\nabla \ln q(\hat{x}_{kh})\,dt + \sqrt{2}\,dB_t$ for $t \in [kh, (k+1)h)$

TRUE: $dx_t = -\nabla \ln q(x_t)\,dt + \sqrt{2}\,dB_t$

$$KL(\text{TRUE}\,\|\,\text{ALG}) = \frac{1}{4}\mathbb{E}_{\text{TRUE}}\int_0^T \|\nabla \ln q(x_t) - \nabla \ln q(x_{kh})\|^2\,dt$$

$$\leq \frac{L^2}{4}\mathbb{E}_{\text{TRUE}}\int_0^T \|x_{kh} - x_t\|^2\,dt$$

$$\|x_t - x_{kh}\|^2 = \left\|\int_0^h \nabla \ln q(x_{kh+s})\,ds + \sqrt{2}(B_t - B_{kh})\right\|^2$$

$$\leq 2h\int_0^h \|\nabla \ln q(x_{kh+s})\|^2\,ds + 4\|B_t - B_{kh}\|^2$$

$$\leq \frac{L^2 h}{2} \int_0^T \mathbb{E}_{TRUE}\left[\|\nabla \ln q(x_t)\|^2 dt + 2hd\right]$$