

HW8

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The solution and ideas are based on Gemini and adapt by myself with fully comprehension.

Q1

Show that the sliced score matching (SSM) loss can also be written as

$$L_{SSM} = \mathbb{E}_{x \sim p(x)} \mathbb{E}_{v \sim p(v)} [\|v^T S(x; \theta)\|^2 + 2v^T \nabla_x (v^T S(x; \theta))].$$

Solution

The core idea of SSM is to not match the entire score vectors $S(x; \theta)$ and $\nabla_x \log p(x)$, but to match their one-dimensional projections onto a set of random direction vectors v .

The explicit loss is the expected squared difference between these projections:

$$L_{SSM, explicit}(\theta) = \mathbb{E}_{x \sim p(x)} \mathbb{E}_{v \sim p(v)} [(v^T S(x; \theta) - v^T \nabla_x \log p(x))^2]$$

1. Expanding the squared term

For simplicity, let's omit the function arguments $(x; \theta)$

$$\begin{aligned} L_{SSM, explicit} &= \mathbb{E}_{x,v} [(v^T S - v^T \nabla_x \log p(x))^2] \\ &= \mathbb{E}_{x,v} [(v^T S)^2 - 2(v^T S)(v^T \nabla_x \log p(x)) + (v^T \nabla_x \log p(x))^2] \end{aligned}$$

Using the linearity of expectation, we can break this into three terms:

$$L_{SSM, explicit} = \underbrace{\mathbb{E}_{x,v} [(v^T S)^2]}_{\text{Term 1}} - \underbrace{2 \mathbb{E}_{x,v} [(v^T S)(v^T \nabla_x \log p(x))]}_{\text{Term 2}} + \underbrace{\mathbb{E}_{x,v} [(v^T \nabla_x \log p(x))^2]}_{\text{Term 3}}$$

Now let's analyze each term:

- **Term 1** is already present in our target expression. We don't need to change it.
- **Term 2** is the one we need to rewrite.
- **Term 3** does not depend on the parameter θ . Therefore, it is a constant C.

2. Rewriting the second term

First, let's fix a random vector v and only consider the expectation over x :

$$\mathbb{E}_{x \sim p(x)} [(v^T S)(v^T \nabla_x \log p(x))]$$

We use the identity $\nabla_x \log p(x) = \frac{\nabla_x p(x)}{p(x)}$:

$$= \int_{\mathbb{R}^d} p(x) \left((v^T S(x)) \left(v^T \frac{\nabla_x p(x)}{p(x)} \right) \right) dx = \int_{\mathbb{R}^d} (v^T S(x))(v^T \nabla_x p(x)) dx$$

Since $v^T S$ is a scalar, let the scalar function be $h(x) = v^T S(x)$. The integral is $\int h(x)(v^T \nabla_x p(x)) dx$. Let's write out the dot product $v^T \nabla_x p(x) = \sum_i v_i \frac{\partial p(x)}{\partial x_i}$.

$$= \int h(x) \left(\sum_i v_i \frac{\partial p(x)}{\partial x_i} \right) dx = \sum_i v_i \int h(x) \frac{\partial p(x)}{\partial x_i} dx$$

2.1 Integration by parts

Now, we focus on the integral inside the summation, which is a one-dimensional integral with respect to the variable x_i . We apply the standard integration by parts formula:

$$\int u dv = uv - \int v du$$

For the integral $\int h(x) \frac{\partial p(x)}{\partial x_i} dx_i$, we set:

- $u = h(x)$
- $dv = \frac{\partial p(x)}{\partial x_i} dx_i$

This gives us:

- $du = \frac{\partial h(x)}{\partial x_i} dx_i$
- $v = \int \frac{\partial p(x)}{\partial x_i} dx_i = p(x)$

Plugging these into the formula, we get:

$$\int_{-\infty}^{+\infty} h(x) \frac{\partial p(x)}{\partial x_i} dx_i = \underbrace{[h(x)p(x)]_{x_i=-\infty}^{x_i=+\infty}}_{\text{Boundary Term}} - \int_{-\infty}^{+\infty} p(x) \frac{\partial h(x)}{\partial x_i} dx_i$$

The crucial step is to analyze the Boundary Term. A fundamental property of any well-behaved probability density function $p(x)$ defined over \mathbb{R}^d is that it must vanish at infinity. That is:

$$\lim_{\|x\| \rightarrow \infty} p(x) = 0$$

We also assume that $S(x)$ (and $h(x)$) does not grow faster than $p(x)$ decays. Thus, the product $h(x)p(x)$ goes to zero at the boundaries:

$$\lim_{x_i \rightarrow \pm\infty} (h(x)p(x)) = 0$$

Therefore, the boundary term is $0 - 0 = 0$ and then vanishes. This simplifies our result to:

$$\int h(x) \frac{\partial p(x)}{\partial x_i} dx_i = - \int p(x) \frac{\partial h(x)}{\partial x_i} dx_i$$

Substituting this back into the sum:

$$= \sum_i v_i \left(- \int p(x) \frac{\partial h(x)}{\partial x_i} dx \right) = - \int p(x) \left(\sum_i v_i \frac{\partial h(x)}{\partial x_i} \right) dx$$

The term $\sum_i v_i \frac{\partial h(x)}{\partial x_i}$ is exactly the dot product $v^T \nabla_x h(x)$.

$$= - \int p(x) (v^T \nabla_x h(x)) dx = - \mathbb{E}_{x \sim p(x)} [v^T \nabla_x h(x)]$$

Now, substitute $h(x) = v^T S(x)$ back in:

$$\mathbb{E}_{x \sim p(x)} [(v^T S)(v^T \nabla_x \log p(x))] = - \mathbb{E}_{x \sim p(x)} [v^T \nabla_x (v^T S(x))]$$

So we rewrite the term 2 into:

$$\text{New Term 2} = -2 \mathbb{E}_{x \sim p(x)} [v^T \nabla_x (v^T S(x))]$$

3. Putting it all together

Let's go back to our expanded loss function:

$$\begin{aligned} L_{SSM} &= \text{Term 1} + \text{New Term 2} + \text{Term 3} \\ &= \mathbb{E}_{x,v} [(v^T S)^2] - 2 (-\mathbb{E}_{x,v} [v^T \nabla_x (v^T S)]) + C \\ &= \mathbb{E}_{x,v} [(v^T S(x; \theta))^2 + 2v^T \nabla_x (v^T S(x; \theta))] + C \end{aligned}$$

Since minimizing $L_{SSM}(\theta) + C$ with respect to θ is equivalent to minimizing $L_{SSM}(\theta)$, we can omit the constant C . Thus, we get the desired result.

Q2

Briefly explain SDE.

Solution

Stochastic differential equation (SDE)

An SDE models a system that evolves over time under both deterministic drift and random diffusion.

- **SDE General Form:**

$$dx_t = \underbrace{f(x_t, t)}_{\text{Drift}} dt + \underbrace{G(x_t, t)}_{\text{Diffusion}} dW_t$$

- * x_t : The state of the system at time t .
- * $f(x_t, t)$: The **drift** coefficient, a vector describing the deterministic trend of the process.
- * $G(x_t, t)$: The **diffusion** coefficient, a matrix defining the magnitude of the random noise.
- * W_t : A standard **Wiener process** (or Brownian motion).

- **Integral Form (Ito Integral):**

$$x_t = x_0 + \int_0^t f(x_s, s) ds + \int_0^t G(x_s, s) dW_s$$

The second integral, $\int G dW_s$, is an Ito integral, defined as a limit of sums over random increments of W_t .

Wiener Process (Brownian Motion) W_t

A continuous stochastic process modeling random motion.

1. Start at origin: $W_0 = 0$.
2. Increments: Has independent and stationary Gaussian increments, where $W_{t+\Delta t} - W_t \sim N(0, \Delta t I)$.
3. Paths: Sample paths are continuous but nowhere differentiable with probability 1.

Numerical Simulation: Euler-Maruyama Method

SDEs are typically solved numerically by discretizing time into steps of size Δt .

- **Update Rule:**

$$X_{n+1} = X_n + f(X_n, t_n) \Delta t + G(X_n, t_n) \sqrt{\Delta t} Z_n$$

where Z_n are independent random variables drawn from a standard normal distribution, $N(0, I)$.

Key Examples

- **Brownian Motion with Drift:**

$$dx_t = \mu dt + \sigma dW_t$$

Solution $x(t) \sim N(x_0 + \mu t, \sigma^2 t)$. It follows a linear trend with added random noise.

- **Ornstein-Uhlenbeck (OU) process:**

$$dx_t = -\beta x_t dt + \sigma dW_t$$

A **mean-reverting** process. The drift term $-\beta x_t$ acts as a restoring force, pulling the process back towards its mean (in this case, 0).