
Nonparametric variational inference via score matching

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1 Introduction

This sheet details a new proposed method for variational inference. The method, score matching, is widely used in high dimensional density estimation, and we first explain how it is used in that context. Let us have data $z_1, \dots, z_n \sim_{i.i.d.} \mathbb{P}$, where \mathbb{P} is a distribution with density p . We wish to estimate p . Score matching seeks a density q to minimize a Fisher divergence, defined via

$$\mathcal{L}(q) = \mathbb{E}_p \|\nabla_z \log p(z) - \nabla_z \log q(z)\|_2^2. \quad (1)$$

Notice that in $\nabla_z \log q(z)$, any normalizing constant disappears. Thus, this method is appealing for density estimation because it does not require estimation of a normalizing constant,

which is typically intractable in high dimensions. By a simple argument using integration by parts, this objective simplifies to something that we can easily optimize in q ; see Lemma 5.1. For exponential families, it further simplifies into a nice quadratic; see Lemma 5.2. It has been used in high dimensional density estimation where the normalizing constant is not computable, for example, in graphical models, c.f. Hyvarinen (2005), Lin *et al.* (2016), and Janofsky (2015).

2 Score matching for posterior inference

We notice that the objective (1) is usable for posterior inference. Suppose we observe data x generated according to the conditional density $p(x|z)$. Associated to x is a latent variable z with a prior $p(z)$. We seek the posterior density:

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)}.$$

But typically $p(x)$ is not tractable. But minimizing the following objective in q would not require us to have $p(x)$, since $\nabla_z \log p(z|x) = \nabla_z \log p(x|z) + \nabla_z \log p(z)$.

$$\mathcal{L}(q) = \mathbb{E}_{p(z|x)} \|\nabla_z \log q(z|x) - \nabla_z \log p(z|x)\|_2^2.$$

But is this something we can minimize? It turns out that it is. Suppose we assume that $p(z|x) \propto e^{f(z|x)}$, i.e., the posterior has an exponential family form. Suppose further that $f(z|x) = f_x(z) = \gamma^\top \phi(z)$, where $\gamma \in \mathbb{R}^K$ and $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^K$. Then just as in Lemma 5.2, the objective simplifies to:

$$\int_z p(z|x) \left(\frac{1}{2} \gamma' A(z) \gamma + \gamma' k(z) \right) dz \quad (2)$$

which has optimal solution

$$\hat{\gamma} = \bar{A}^{-1} \bar{k} \quad (3)$$

where

$$\begin{aligned} \bar{A} &= \int p(z, x) A(z) dz \\ \bar{k} &= \int p(z, x) k(z) dz \end{aligned}$$

where \bar{A}, \bar{k} are defined below. Note the following key fact: the optimal solution requires integrals only over $p(z, x)$, not over $p(z|x)$, since the form in (3) allows the normalizing constant $p(x)$ to drop out! Thus this is something we can optimize.

But here are some important caveats. It actually is difficult to compute these integrals over the joint density. If we could, computing $p(x)$ wouldn't be a problem in the first place. We have considered importance-sampling. One issue is that often $p(x|z)$ is extremely small if n is large. Another is that, e.g., in the Gaussian family case, we still need $p(x)$; see Example 1. In fact, in any case where the first or second derivatives are constant, again, we would just be computing $p(x)$ via importance sampling.

However, we do implement this algorithm in some simple cases; see the script at [Non-parametric variational inference via score matching](#).

3 Alternative algorithms

3.1 \mathbb{E}_q and Kernel density estimation

We here discuss other variants of the score-matching objective for variational inference. [Ranganath et al. \(2016\)](#) use the same objective as in (1), but with the expectation taken over the density q :

$$\mathcal{L}(q) = \mathbb{E}_q \|\nabla_z \log q(z) - \nabla_z \log p(z)\|_2^2. \quad (4)$$

They re-express it in operator variational inference form, i.e., in the form $\mathbb{E}_q O(f, p)$. They use the Langevin Stein operator and iterate over optimizing the function f and the density q ; see Section 7 for details. This has the weakness that it requires a min-max type of optimization. An equivalence between the objectives (4) and (1) is in Lemma 7.3.

Instead of the approach in [Ranganath et al. \(2016\)](#), we might directly optimize (4). We do this via the reparametrization trick. We posit a sampling form for q ; i.e., we generate Gaussian noise ξ , then feed it through a multilayer perceptron to generate samples from z from q . That is, we draw

$$\begin{aligned} z_{0i} &\sim N(0, I_{d_0}) \\ z_i &= f_\phi(z_{0i}), \end{aligned} \quad (5)$$

where f_ϕ is some multilayer perceptron function. Now given this sampling form for q , we cannot write down an exact formula for $q(z)$; since this transformation of ξ is not invertible, we cannot use the change of variable density formula. Thus, it seems impossible to optimize (4) directly since it requires the form of q since we take $\nabla_z \log q(z)$. However, we propose to imitate the score matching method in [Saremi et al. \(2018\)](#) to get around this difficulty. This method is to approximate the form of q using an approximate kernel density estimator. For each data point z_i , we generate Gaussian samples $\xi_{i1}, \dots, \xi_{im}$. [Saremi et al. \(2018\)](#) then use:

$$\nabla_\xi \log q(\xi) \approx \sum_{j=1}^m (z_i - \xi_{ij})$$

Note that a kernel density estimator using a Gaussian kernel would have the form:

$$q(z_i) \propto \sum_{j=1}^m e^{-\|z_i - \xi_{ij}\|_2^2 / 2\sigma^2}$$

So the gradient above is approximately the gradient of the log of this. We optimize the parameters of the likelihood using EM. So our full optimization is:

$$\max_{\phi} \sum_{i=1}^n \left\| \sum_{j=1}^m f_\phi(z_{0i}) - \xi_{ij} - \nabla_z \log p_\theta(x_i, f_\phi(z_{0i})) \right\| \leftarrow \text{Posterior optimization}$$

$$\max_{\theta} \sum_{i=1}^n \log p_\theta(x_i, f(z_{0i})) \leftarrow \text{Likelihood optimization}$$

We carry this out in Tensorflow.

3.2 Ratio matching

We propose one other alternative. First, notice the following. For small h ,

$$\nabla_z \log q(z) \approx \frac{\log q(z+h) - \log q(z)}{h} = \frac{1}{h} \log \frac{q(z+h)}{q(z)}$$

This is the basis of ratio-matching, which approximates score matching using the above representation of the derivative. Draw samples z_1, z_2 from a sampling form q , as in (5), and optimize

$$\mathbb{E}_q \left\| \log \frac{q(z_1)}{q(z_2)} - \log \frac{p(x, z_1)}{p(x, z_2)} \right\|_2^2. \quad (6)$$

This imitates the method of Hyvarinen (2007). To begin, we use a Gaussian form for q . Since we can sample from this, we use the reparametrization trick to estimate the integral in (6).

4 Examples

Example 1 (Score-matching with \mathbb{E}_p for posterior inference when q has Gaussian form). Suppose q has form $N(\mu_x, \Sigma_x)$ where $\mu_x \in \mathbb{R}^d, \Sigma_x \in \mathbb{R}^{d \times d}$. Let our prior $p(z)$ be the $N(0, I_d)$ density. Note that we could have $d \gg n$. We have $q(z) \propto e^{g(z)}$ where

$$g(z) = \gamma' \phi(z)$$

where $K = 2d$ and

$$\begin{aligned} \gamma &= (\Sigma^{-1}, \Sigma^{-1}\mu)^T \\ \phi(z) &= \left(-\frac{1}{2}zz', z \right)^T \end{aligned}$$

So (for $d = 1$, to keep it simple):

$$\begin{aligned} \frac{\partial \phi(z)}{\partial z} &= (-z, 1)^T \\ \frac{\partial^2 \phi(z)}{\partial z^2} &= (1, 0)^T \end{aligned}$$

We have $A(z) \in \mathbb{R}^{2d \times 2d}$. Let e.g. z^2 indicate (z_1^2, \dots, z_d^2) . We have

$$\begin{aligned} A(z) &= \begin{pmatrix} \text{diag}(z^2) & \text{diag}(-z) \\ \text{diag}(-z) & \text{diag}(1) \end{pmatrix} \text{ and} \\ k(z) &= (\text{rep}(-1, d), \text{rep}(0, d))^T \end{aligned}$$

Each submatrix is in $\mathbb{R}^{d \times d}$. We parameterize γ via B ; it is some multi-layer non-linear function with many parameters B . Our objective, written as a sum, is

$$\mathbb{E}_{p(z|x)} \left(\sum_{j \leq d} \gamma_{1j}^2 z_j^2 - \sum_{j \leq d} \gamma_{2j} \gamma_{1j} z_j + \sum_{j \leq d} \gamma_{2j}^2 - \sum_{j \leq d} \gamma_{1j} \right)$$

Note that as noted in ? and [Lin et al. \(2016\)](#), there are closed-form solutions of μ, Σ . To see it, note that if $q(z)$ is $N(\mu, \Sigma)$,

$$\log q(z) \propto \frac{-(z - \mu)' \Sigma^{-1} (z - \mu)}{2}$$

So the score-matching objective is

$$\frac{1}{2} \|\nabla_z \log q(z)\|_2^2 + \Delta_z \log q(z) = \frac{1}{2} \|\Sigma^{-1} (z - \mu)\|_2^2 + \text{tr}(\Sigma^{-1})$$

We can directly obtain:

$$\begin{aligned} \hat{\mu} &= \mathbb{E}_{p(z|x)} z \\ \hat{\Sigma}_i &= \mathbb{E}_{p(z|x)} (z - \hat{\mu})(z - \hat{\mu})' \end{aligned}$$

While this is estimable for density estimation, it requires the posterior for us. Why does this happen when we can still not require $p(x)$ if we compute the exponential family parameter? Notice that e.g. in the simple $d = 1$ case, the quadratic we'd obtain for score-matching is:

$$\gamma' \mathbb{E}_{p(z|x)} \begin{pmatrix} z^2 & z \\ z & 1 \end{pmatrix} \gamma - \gamma' \mathbb{E}_{p(z|x)} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Optimizing this allows us to remove the $p(x)$, but notice that then, we optimize in $\gamma \gamma' \bar{A} \gamma' - \gamma' \bar{k}$, the usual thing, where

$$\bar{k} = \begin{pmatrix} p(x) \\ 0 \end{pmatrix}$$

Now again we can approximate $p(x)$ via importance sampling, but we do have to approximate it either way.

5 Basics of score matching with \mathbb{E}_p

Lemma 5.1 (Score-matching simplifies to something simple using integration by parts). *Let $\hat{q} = \text{argmin}_q \mathcal{L}(q)$ where $\mathcal{L}(q)$ is as above. Then*

$$\begin{aligned} \hat{q} &= \text{argmin}_q \int_z p(z|x) \sum_{i \leq d} \frac{1}{2} \left(\frac{\partial \log q(z)}{\partial z_i} \right)^2 + \frac{\partial^2 \log q(z)}{\partial z_i^2} dz \\ &= \text{argmin}_q \int_z p(z|x) \left(\frac{1}{2} \|\nabla \log q\|_2^2 + \Delta \log q \right) dz \end{aligned}$$

Proof. I just write this for one dimension. For an extension to higher dimensions, see [Hyvarinen \(2005\)](#). I sometimes write $p'(z)$ instead of $\frac{\partial p(z)}{\partial z}$.

$$\int p(z) \left(\frac{\partial \log p(z)}{\partial z} - \frac{\partial \log q(z)}{\partial z} \right)^2 dz \stackrel{c}{=} \int p(z) \left(\frac{\partial \log q(z)}{\partial z} \right)^2 - 2 \int p'(z) \frac{\partial \log q(z)}{\partial z}$$

And using integration by parts,

$$\int p'(z) \frac{\partial \log q(z)}{\partial z} \stackrel{c}{=} - \int p(z) \frac{\partial^2 q(z)}{\partial z^2}$$

□

Lemma 5.2 (The score-matching objective simplifies into a nice quadratic for exponential families.). *Let*

$$q(z) = \frac{e^{g(z)}}{\int e^{g(z)} dz}$$

Suppose $g : \mathbb{R}^d \rightarrow \mathbb{R}$, with

$$g(z) = \gamma' \phi(z)$$

where $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^K$ and $\gamma \in \mathbb{R}^K$. Write $\phi(z) = (\phi_1(z), \dots, \phi_K(z))'$. Estimating q means estimating γ . Define

$$\begin{aligned} \frac{\partial \phi(z)}{\partial z_i} &= \left(\frac{\partial \phi_1(z)}{\partial z_i}, \dots, \frac{\partial \phi_K(z)}{\partial z_i} \right)^T \\ \frac{\partial^2 \phi(z)}{\partial z_i^2} &= \left(\frac{\partial^2 \phi_1(z)}{\partial z_i^2}, \dots, \frac{\partial^2 \phi_K(z)}{\partial z_i^2} \right)^T \end{aligned}$$

For a non-bounded density (the second line is for an exponential family), the objective is, as in [Janofsky \(2015\)](#) and [Hyvarinen \(2007\)](#):

$$\begin{aligned} h_\gamma(z) &= \sum_{i \leq d} \frac{1}{2} \left(\frac{\partial g(z)}{\partial z_i} \right)^2 + \frac{\partial^2 g(z)}{\partial z_i^2} \\ &= \sum_{i \leq d} \frac{1}{2} \left(\gamma' \frac{\partial \phi(z)}{\partial z_i} \right)^2 + \gamma' \frac{\partial^2 \phi(z)}{\partial z_i^2} \end{aligned}$$

Now here are the definitions of A, k . Note $A \in \mathbb{R}^{K \times K}, k \in \mathbb{R}^K$. For a non-bounded density:

$$\begin{aligned} k(z) &= \sum_{i \leq d} \frac{\partial^2 \phi(z)}{\partial z_i^2} \\ A(z) &= \sum_{i \leq d} \frac{\partial \phi(z)}{\partial z_i} \frac{\partial \phi(z)}{\partial z_i}' \end{aligned}$$

5.1 Bounded density

For a bounded density, score matching has a slightly different objective. See [Janofsky \(2015\)](#) for more details.

$$\begin{aligned}
k_1(z) &= \sum_{i \leq d} 2(2z_i - 1)z_i(1 - z_i) \frac{\partial \phi(z)}{\partial z_i} \\
k_2(z) &= \sum_{i \leq d} z_i^2(1 - z_i)^2 \frac{\partial^2 \phi(z)}{\partial z_i^2} \\
k(z) &= k_1(z) - k_2(z) \\
A(z) &= \sum_{i \leq d} \frac{\partial \phi(z)}{\partial z_i} \frac{\partial \phi(z)}{\partial z_i}' z_i^2(1 - z_i)^2
\end{aligned}$$

For a bounded density (the second line is for an exponential family), the objective is:

$$\begin{aligned}
h_\gamma(z) &= \sum_{i \leq d} \frac{1}{2} \left(\frac{\partial g(z)}{\partial z_i} z_i(1 - z_i) \right)^2 - 2(2z_i - 1)z_i(1 - z_i) \frac{\partial g(z)}{\partial z_i} + z_i^2(1 - z_i)^2 \frac{\partial^2 g(z)}{\partial z_i^2} \\
&= \sum_{i \leq d} \left(\gamma' \frac{\partial \phi(z)}{\partial z_i} z_i(1 - z_i) \right)^2 - 2(2z_i - 1)z_i(1 - z_i) \gamma' \frac{\partial \phi(z)}{\partial z_i} + z_i^2(1 - z_i)^2 \gamma' \frac{\partial^2 \phi(z)}{\partial z_i^2}
\end{aligned}$$

In one dimension, and for $z \in [0, 1]$, this simplifies to the following. Let $\phi : [0, 1] \rightarrow \mathbb{R}^K$.

$$\begin{aligned}
h_\gamma(z) &= \frac{1}{2} \left(\frac{\partial g(z)}{\partial z} z(1 - z) \right)^2 - 2(2z - 1)z(1 - z) \frac{\partial g(z)}{\partial z} + z(1 - z) \frac{\partial^2 g(z)}{\partial z^2} \\
&= \frac{1}{2} z^2(1 - z)^2 \gamma' A(z) \gamma - 2(2z - 1)z(1 - z) \gamma' k_1(z) + z^2(1 - z)^2 \gamma' k_2(z)
\end{aligned}$$

where

$$\begin{aligned}
k_1(z) &= \left(\frac{\partial \phi_1(z)}{\partial z}, \dots, \frac{\partial \phi_K(z)}{\partial z} \right)' \\
k_2(z) &= \left(\frac{\partial^2 \phi_1(z)}{\partial z^2}, \dots, \frac{\partial^2 \phi_K(z)}{\partial z^2} \right)' \\
k(z) &= k_1(z) - k_2(z) \\
A(z) &= k_1(z) k_1(z)'
\end{aligned}$$

6 Basics of score matching with \mathbb{E}_q

The following lemma shows that the score-matching objective (4) decomposes into two components: a component matching q to p , and a component restricting q to be reasonably smooth. Thus the score-matching divergence decomposes in a similar manner as the KL divergence.

Lemma 6.1. Suppose $q(z) = \exp(f(z) - \Psi)$ where Ψ is the normalizing constant. Let $\mathcal{L}(q) = \mathbb{E}_q \|\nabla_z \log p - \nabla_z \log q\|_2^2$. Then

$$\mathcal{L}(q) =^c \frac{1}{2} \mathbb{E}_q \|\nabla_z \log p(z, x)\|_2^2 + \mathbb{E}_q \Delta \log p(z, x) + \mathbb{E}_q \|\nabla_z f(z)\|_2^2$$

Proof. [Only in one dimension for now.]

$$\mathcal{L}(q) = \int q(z) \left(\frac{\partial}{\partial z} \log p \right)^2 - 2 \int q(z) \frac{q'(z)}{q(z)} \frac{p'(z)}{p(z)} + \int q(z) \left(\frac{\partial}{\partial z} \log q(z) \right)^2$$

The third term is $\mathbb{E}_q f'(z)^2$. And for the middle term, using integration by parts,

$$\int q(z) \frac{q'(z)}{q(z)} \frac{p'(z)}{p(z)} = \int q'(z) \frac{\partial}{\partial z} \log p(z) =^c - \int q(z) \frac{\partial^2}{\partial z^2} \log p(z)$$

□

The following lemma shows that when we assume $q(z)$ is a Gaussian density, the score-matching objective as in (4) reduces to the Laplace method as in Wang & Blei (2013). In retrospect, this is obvious by Lemma 7.1; since we assume a Gaussian form for the model, as long as we are optimizing over \mathcal{Q} that includes Gaussian densities, we should obtain “the right thing.” But this is nice as a sanity check.

Lemma 6.2. Let $z \in \mathbb{R}^d$. Let $f(z) := \log p(z)$ and suppose for any z_0 ,

$$f(z) \approx f(z_0) + \nabla f(z_0)^T (z - z_0) + \frac{1}{2} (z - z_0)^T \nabla^2 f(z_0) (z - z_0)$$

. Let $z^* \in \arg\max f(z)$. Let \mathcal{Q} be $N(\lambda, V)$ densities. Let $\hat{q} = \arg\min_{q \in \mathcal{Q}} \mathbb{E}_q \|\nabla_z \log p - \nabla_z \log q\|_2^2$. Then \hat{q} is the $N(\hat{\lambda}, \hat{V})$ density with

$$\begin{aligned} \hat{\lambda} &= z^* \\ \hat{V} &= -\nabla^2 f(z^*) \end{aligned}$$

Proof. Let z^* be a mode of f , i.e., $\nabla_z f(z^*) = 0$. Then

$$f(z) \approx f(z_0) + \frac{1}{2} (z - z^*)^T \nabla^2 f(z^*) (z - z^*)$$

So

$$\nabla_z f(z) \approx \nabla^2 f(z^*) (z - z^*)$$

Let q be the $N(\lambda, V)$ density where $\lambda \in \mathbb{R}^d$ and $V \in \mathbb{R}^{d \times d}$; λ and V are the parameters to be optimized. Now $\nabla_z \log q(z) = -V^{-1}(z - \lambda)$. Now $z = V^{1/2}z_0 + \lambda$, where $z_0 \sim N(0, I_p)$. So

$$\begin{aligned} \mathcal{L}(q) &= \mathbb{E}_q \|\nabla_z \log q(z) - \nabla_z \log p(z)\|_2^2 \\ &= \mathbb{E}_{z_0 \sim N(0, I_p)} \|-V^{-1/2}z_0 - \nabla^2 f(z^*)(V^{1/2}z_0 + \lambda - z^*)\|_2^2 \\ &= \mathbb{E}_{z_0} \|(-V^{-1/2} - \nabla^2 f(z^*)V^{1/2})z_0 - \nabla^2 f(z^*)(\lambda - z^*)\|_2^2 \\ &= \mathbb{E}_{z_0} \|(-V^{-1/2} - \nabla^2 f(z^*)V^{1/2})z_0\|_2^2 + \|\nabla^2 f(z^*)(\lambda - z^*)\|_2^2 \\ &= \|V^{-1/2} + \nabla^2 f(z^*)V^{1/2}\|_F^2 + \|\nabla^2 f(z^*)(\lambda - z^*)\|_2^2 \end{aligned}$$

Optimizing in λ yields:

$$\hat{\lambda} = z^*$$

Let $M = \nabla^2 f(z^*)$. Let's do one dimension to check:

$$v^{-1/2} + mv^{1/2} = \frac{1 + mv}{\sqrt{v}}$$

And

$$\left(\frac{1 + mv}{\sqrt{v}}\right)^2 = \frac{1 + 2mv + m^2v^2}{v} = \frac{1}{v} + 2m + m^2v$$

Now

$$\frac{\partial}{\partial v} \left(\frac{1}{v} + 2m + m^2v \right) = -\frac{1}{v^2} + m^2$$

Setting this equal to zero yields:

$$V^2 = M^{-2} \Rightarrow V = \pm M^{-1}$$

which is exactly the Laplace method solution. \square

Example 2 (Lemma 6.1 in the Gaussian case). *Consider the objective (4). In the case where q is Gaussian, as in, Lemma 6.2, we can see that only optimizing the first two terms of the score-matching objective would lead to a terribly sharp q (with zero variance). The final term (the penalty on the smoothness of q) forces more smoothness. Let the setting be as in Lemma 6.2: q is the $N(\lambda, V)$ and the Taylor expansion for $\log p(x, z)$ holds. Now,*

$$\begin{aligned} \frac{1}{2} \mathbb{E}_q \|\nabla_z \log p(z, x)\|_2^2 + \mathbb{E}_q \Delta \log p(z, x) &= \frac{1}{2} \mathbb{E}_q (z - z^*)^T (\nabla^2 f(z^*))^2 (z - z^*) - \mathbb{E}_q \nabla^2 f(z^*) \\ &=^c \frac{1}{2} \text{tr} \left(V^T (\nabla^2 f(z^*))^2 V \right) + (\lambda - z^*)^T (\nabla^2 f(z^*))^2 (\lambda - z^*) \end{aligned}$$

which would be optimized by setting $\hat{\lambda} = z^*$ and $\hat{V} = 0$. But we have the penalty:

$$\mathbb{E}_q \|\nabla \log q\|_2^2 = \text{tr}(V^{-1})$$

Due to this penalty, we end up with a reasonable q .

7 Relationship between score-matching, Stein discrepancy, and OVI

Let $\psi_p(z) = \frac{\partial \log p(z)}{\partial z} = p'(z)/p(z)$ and similarly for $\psi_q(z)$. Let $\Delta p = \frac{\partial^2 \log p(z)}{\partial z^2}$. Let $O^{p,q}$ be some operator depending on p, q . I will use the following form for exponential families in z :

$$p(z) = \exp(\gamma \phi(z) - \Psi(\gamma)) \tag{7}$$

The authors of [Ranganath *et al.* \(2016\)](#) propose to optimize following variational objective in q :

$$\sup_{f \in \mathcal{F}} |\mathbb{E}_{q(z)}(O_{LS}^p f)(z)| \quad (8)$$

where

$$O_{LS}^p f = \psi_p f + \nabla f \quad (9)$$

Just as in the proof of Lemma 7.2, the objective (8) is

$$\sup_{f \in \mathcal{F}} |\mathbb{E}_q O_{LS}^p f| = \sup_{f \in \mathcal{F}} \mathbb{E}_{q(z)} (\psi_q(z) - \psi_p(z)) f(z) \quad (10)$$

$$= \mathbb{E}_{q(z)} (\psi_q(z) - \psi_p(z))^2 \quad (11)$$

i.e., their objective is the score-matching objective with expectation over q . But if we use a specific class \mathcal{F} as in the following lemma, this becomes the usual score-matching objective with expectation over p .

The following lemma shows that (8) is valid in that it is zero when $q = p$. Of course, when we express the objective as in Lemma 7.2, this becomes even more obvious.

Lemma 7.1. *Assume q is zero at the boundaries of the sample space. Then*

$$\mathbb{E}_{q(z)} (\psi_q f(z) + f'(z)) = 0$$

Proof. First, by the product rule,

$$\mathbb{E}_{p(z)} (\psi_q(z) f(z) + f'(z)) = \int_z \frac{p(z)}{q(z)} \frac{\partial (q(z) f(z))}{\partial z} dz$$

Now

$$\int \frac{q(z)}{q(z)} \frac{\partial (q(z) f(z))}{\partial z} dz = \int \frac{\partial}{\partial z} (q(z) f(z)) dz = q(\infty) f(\infty) - q(-\infty) f(-\infty) = 0$$

under some assumptions on q, f . □

Lemma 7.2 (Equivalence of score-matching and Stein discrepancy under specific \mathcal{G}). *Let \mathcal{G} be a class of functions of the form $g(z) = \psi_q(z) f(z) + f'(z)$, for f in some class of functions \mathcal{F} . Then*

$$\sup_{g \in \mathcal{G}} |\mathbb{E}_{p(z)} g(z)| = \sup_{f \in \mathcal{F}} |\mathbb{E}_{p(z)} (\psi_q(z) f(z) + f'(z))| = \mathbb{E}_p (\psi_p - \psi_q)^2$$

Proof. By Lemma 7.1, $\mathbb{E}_{p(z)} \psi_p(z) f(z) + f'(z) = 0$. So

$$\begin{aligned} \sup_{g \in \mathcal{G}} |\mathbb{E}_{p(z)} g(z)| &= \sup_{f \in \mathcal{F}} |\mathbb{E}_{p(z)} (\psi_q(z) f(z) + f'(z) - \psi_p(z) f(z) - f'(z))| \\ &= \sup_{f \in \mathcal{F}} |\mathbb{E}_p (\psi_q - \psi_p) f| \end{aligned}$$

And this is maximized when $f(z) = \psi_q(z) - \psi_p(z)$. □

Lemma 7.3. *Let \mathcal{F} be a class of functions of the form (assuming the densities are positive everywhere):*

$$f(z) = \frac{p(z)}{q(z)} h(z) \quad (12)$$

for $h(z)$ in some class of functions \mathcal{H} . Then

$$\sup_{f \in \mathcal{F}} |\mathbb{E}_q O_{LS}^p f| = \sup_{h \in \mathcal{H}} |\mathbb{E}_p O_{LS}^q h|$$

Proof. This is clear if we use the representation in (10) and apply Lemma 7.2. That is,

$$\sup_{f \in \mathcal{F}} |\mathbb{E}_q O_{LS}^p f| = \sup_{f \in \mathcal{F}} \mathbb{E}_q (\psi_q - \psi_p) f = \sup_{h \in \mathcal{H}} \mathbb{E}_q \frac{p}{q} (\psi_q - \psi_p) h = \sup_{h \in \mathcal{H}} \mathbb{E}_p (\psi_q - \psi_p) h = \sup_{h \in \mathcal{H}} |\mathbb{E}_p O_{LS}^q h|$$

Alternatively (this is a sanity check):

$$\begin{aligned} \sup_{f \in \mathcal{F}} |\mathbb{E}_q O_{LS}^p f| &= \sup_{f \in \mathcal{F}} |\mathbb{E}_q (\psi_p(z) f(z) + f'(z))| \\ &= \sup_{h \in \mathcal{H}} \left| \int q(z) \frac{p'(z)}{p(z)} \frac{p(z)}{q(z)} h(z) + \int q(z) \left(\frac{q(z)p'(z) - p(z)q'(z)}{q(z)^2} h(z) + \frac{p(z)}{q(z)} h'(z) \right) \right| \\ &= \sup_{h \in \mathcal{H}} \left| \int p'(z) h(z) + \int p'(z) h(z) - \int \frac{q'(z)}{q(z)} p(z) h(z) + \int p(z) h'(z) \right| \\ &= \sup_{h \in \mathcal{H}} \left| \int 2(p'(z) h(z) + p(z) h'(z)) - \int p(z) h'(z) - \int \frac{q'(z)}{q(z)} p(z) h(z) \right| \\ &= \sup_{h \in \mathcal{H}} |\mathbb{E}_p (\psi_q(z) h(z) + h'(z))| \end{aligned}$$

since $p'(z)h(z) + p'(z)h(z) = \frac{\partial(p(z)h(z))}{\partial z}$, which has integral zero by Lemma 7.1. \square

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