Abstract

Truncated densities are probability density functions defined on truncated input domains. These densities share the same parametric form with their non-truncated counterparts up to a normalization term. However, normalization terms usually cannot be obtained in closed form for these distributions, due to complicated truncation domains. Score Matching is a powerful tool for fitting parameters in unnormalized models. However, it cannot be straightforwardly applied here as boundary conditions used to derive a tractable objective are usually not satisfied by truncated distributions. In this paper, we propose a maximally weighted Score Matching objective function which takes the geometry of the truncation boundary into account when fitting unnormalized density models. We show the weighting function that maximizes the objective function can be constructed easily and the boundary conditions for deriving a tradable objective are satisfied. Experiments on toy datasets and Chicago crime dataset show promising results.

1 Introduction

In many applications, the window of observation is limited and instead of a “full picture”, we can only observe a truncated dataset. For example, a police department can only monitor crimes up to the city boundary despite the fact that crimes do not stop at an artificial border; Geolocation tracking data can only be observed up to the coverage mobile signal. Thus the dataset is a skewed representation of actual activities. In many cases, truncation boundary can be very complex. For example, the boundary of city of Chicago is a complex polygon (see Figure 1), which cannot be easily approximated by a bounding box or circle.

Moreover, many statistical models are naturally defined on a bounded domain. For example, Dirichlet distribution is defined on a probability simplex, which is a bounded $d-1$ dimensional hyperplane in a $d$ dimensional space (See Figure 1). Dirichlet distribution is often used as the “prior of probability” in Bayesian modelling, so it only make sense if all dimensions of a random sample adds up to one. Bounded densities are not truncated, but depending on the boundary, the normalization term can also be difficult to compute.

Figure 1: Left: City boundary of Chicago and locations of homicide accidents in 2008 (blue dots), Right: samples from Dirichlet distribution on a 2-simplex.

The key challenge of estimating truncated density model parameters is that most truncated (or bounded) density models do not have a closed-form normalization term, as the normalization takes place in a irregular bounded domain in $\mathbb{R}^d$. This creates a computational issue as the classic Maximum Likelihood Estimation (MLE) requires the evaluation of such a normalization term.

Recent years have seen a new class of estimator, called Score Matching (SM) (Hyvärinen, 2005, 2007; Lyu, 2009) rises in popularity. They estimate parameters by minimizing the Fisher-Hyvaerinen divergence (Lyu, 2009). The divergence is defined using the gradients of log model density and log data density which are taken with respect to the input variable, so the normalization term is eliminated and is not involved in the estimation procedure. Thus SM is a natural candidate for estimating truncated density model parameters.

However, the original SM does not work on truncated models as the regularity conditions needed for deriving a tractable objective function are not satisfied by truncated distributions in general. Hyvärinen (2007) proposed a modification on the original objective function so that SM can handle density functions defined on $\mathbb{R}^d_+$. A more generic SM for handling distributions on $\mathbb{R}^d_+$ has been proposed recently and asymptotic efficiency analysis was performed (Yu et al., 2019). Promising results have been observed on high-dimensional non-negative graphical model structure estimation (Yu et al., 2019).
If the density is truncated in a dimension-wise manner with a lower and upper bound, this problem is known as a doubly truncated distribution estimation (Turnbull 1976, Moreira and de Ua-lvarez 2012). However, few work has been done for more complex truncation domains. We study the problem of truncated parameter estimation using SM by minimizing a maximally weighted SM loss. The weighting function is introduced so the boundary conditions required for deriving a tractable objective function is satisfied. We show the maximizer of the weighting function can be obtained in a closed form and be efficiently evaluated. The derivation of the proposed estimator takes the geometry of the truncation domain into consideration.

Thanks to the flexibility of SM, the proposed algorithm works on a wide range of distributions.

We also provide a few examples of the estimator to show as the truncation boundary expands to infinity, these estimators recover MLEs. Finally, an experiment on Chicago crime dataset is given to demonstrate the usefulness of our method.

2 Problem Formulation

Let us denote a probability density function as \( p_\theta(x) : V \rightarrow \mathbb{R} \). \( V \subseteq \mathbb{R}^d \) and \( \theta \) is the parameter vector of the density function. Without loss of generality, we can write \( p_\theta(x) := \frac{\tilde{p}_\theta(x)}{Z_V(\theta)} \), where \( Z_V(\theta) \) is a normalization term defined as \( Z_V(\theta) := \int_V \tilde{p}_\theta(x)dx \) so that \( p_\theta(x) \) is integrated to 1 over its domain \( V \). \( V \) may be a complicated bounded domain e.g., a polytope in \( \mathbb{R}^d \). In such cases, the normalization term usually does not have a closed form.

Our target is a classic statistical model estimation problem: Suppose \( V \) is given, we want to estimate the parameter \( \theta \) in \( p_\theta(x) \) using a set of observations \( X_q = \{x_i\}_{i=1}^n \) and \( X_q \) contains i.i.d. samples from a data generating distribution \( Q \) with an unknown probability density function \( q(x) : V \rightarrow \mathbb{R} \). The estimate \( \hat{\theta} \) is obtained by minimizing a certain statistical criteria (such as KL-divergence). In this work, we do not particularly care if \( \exists \theta, q(x) = p_\theta(x) \), i.e., the model specification is correct or not.

We also do not restrict the family to which the unnormalized density function belongs. For example, \( \tilde{p}_\theta(x) \) can be a Gaussian density or a positive neural network as long as certain regularity conditions are met.

The first challenge comes from the fact that we need to obtain \( \theta \) using only the unnormalized density model \( \tilde{p}_\theta(x) \) as it is not straightforward to calculate \( Z_V(\theta) \) for a complicated \( V \). Therefore MLE cannot be used as it requires the evaluation of \( Z_V(\theta) \).

A popular tool for estimating unnormalized densities is Score Matching (SM) (Hyvärinen 2005). We introduce SM and one extension then explain why they cannot be readily used to estimate truncated models.

3 Score Matching and Its Generalization

Given a density model \( p_\theta(x) \), SM finds an estimate of \( \theta \) by minimizing the Fisher-Hyvaerinen divergence (Lyò 2009) with respect to \( \theta \)

$$\min_{\theta} \mathbb{E}_q[\nabla_x \log p_\theta(x) - \nabla_x \log q(x)]^2$$

$$= \min_{\theta} \mathbb{E}_q[\nabla_x \log p_\theta(x)]^2 - 2\mathbb{E}_q[\nabla_x \log p_\theta(x) \cdot \nabla_x \log q(x)] + C, \quad (1)$$

where \( \cdot \) is the \( L^2 \) norm and \( C = \mathbb{E}_q[\nabla_x \log q(x)]^2 \) which does not depend on \( \theta \). The key advantage of SM comes from the fact that the normalization term of \( p_\theta(x) \) is not required when evaluating the Fisher-Hyvaerinen divergence as \( \nabla_x \log p_\theta(x) = \nabla_x \log \tilde{p}_\theta(x) \).

Unfortunately, \( \mathbb{E}_q[\nabla_x \log p_\theta(x)]^2 \) is not tractable as we cannot directly evaluate the second term in \( \mathbb{E}_q[\nabla_x \log q(x)] \).

However, it can be shown that

$$\mathbb{E}_q[\nabla_x \log p_\theta(x)]^2 - 2\mathbb{E}_q[\nabla_x \log p_\theta(x), \nabla_x \log q(x)] = \mathbb{E}_q[\nabla_x \log p_\theta(x)]^2 + 2\mathbb{E}_q[\nabla_x^2 \log p_\theta(x)] . \quad (2)$$

The tractable objective \( \mathbb{E}_q[\nabla_x \log p_\theta(x)]^2 \) is due to the following Lemma

Lemma 1. if \( \log q(x) \) is continuously differentiable and \( \log p_\theta(x) \) is twice continuously differentiable w.r.t. \( x \) and \( \lim_{|x| \rightarrow \infty} q(x) \partial_{x_i} \log p_\theta(x) = 0, \forall i \in 1, \ldots, d, \)

$$\mathbb{E}_q[\nabla_x \log p_\theta(x), \nabla_x \log q(x)] = \mathbb{E}_q[\nabla_x^2 \log p_\theta(x)] .$$

The original proof given by [Hyvärinen] is based on fundamental theorem of calculus.

The important regularities here are \( q(x) \partial_{x_i} \log p_\theta(x) \) vanishes as \( x \) tends to infinity and the smoothness of \( \log q(x) \) and \( \log p_\theta(x) \). Many density functions defined on \( \mathbb{R}^d \), such as multivariate Gaussian or Gaussian mixture, satisfy above regularity conditions.

The objective function \( \mathbb{E}_q[\nabla_x \log p_\theta(x)]^2 \) can be easily approximated using \( X_q \):

$$\frac{1}{n} \sum_{i=1}^n \|\nabla_x \log p_\theta(x_i)\|^2 + \frac{2}{n} \sum_{i=1}^n \text{tr} \left[ \nabla_x^2 \log p(x; \theta) \right] .$$

However, when \( p_\theta(x) \) is truncated, i.e., density functions are defined on a bounded subset of \( \mathbb{R}^d \), regularity conditions used to derive Lemma 4 no longer holds in general.

To estimate parameters of density functions defined on \( \mathbb{R}^d \), [Yu et al. 2019] introduced a generalized SM objective function:

$$\mathbb{E}_q[\nabla_x \log p_\theta(x) \circ g(x) - \nabla_x \log q(x) \circ g(x)]^2$$

$$= \mathbb{E}_q[\nabla_x \log p_\theta(x) \circ g(x)]^2 - 2\mathbb{E}_q[\nabla_x \log p_\theta(x) \circ g(x), \nabla_x \log q(x)] + C, \quad (3)$$

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where \( g(x) : \mathbb{R}^d \rightarrow \mathbb{R}^d, g(x) \in \mathcal{G} \circ \) is element-wise product, and \( x^2 \) also works in an element-wise fashion.

\[ \mathcal{G} := \{ g | g \text{ is continuously differentiable and } g(0) = 0 \}. \] (4)

One example in \( \mathcal{G} \) is \( g(x) = x \).

Again, the second term in (3) cannot be directly evaluated due to the existence of \( \nabla_x \log q(x) \). However \( \mathcal{G} \) is specifically chosen so that all important regularity conditions for proving Lemma 1 can hold on \( \mathbb{R}^d_+ \) for some choices of \( p_\theta(x) \) and \( q(x) \). We can now have an analogue to Lemma 1:

**Lemma 2.** If \( \log q(x), g(x) \) are continuously differentiable and \( \log p_\theta(x) \) is twice continuously differentiable w.r.t. \( x \) on \( \mathbb{R}^d_+ \) and

\[ \lim_{|x_i| \rightarrow 0^+, |x_i| \rightarrow \infty} g_i^2(x)q(x)\partial_{x_i} \log p_\theta(x) = 0, \forall i, \]

then

\[ \mathbb{E}_q(\nabla_x \log p_\theta \circ g^2, \nabla_x \log q) = -\mathbb{E}_q \sum_{i=1}^d \partial_{x_i} (g_i^2 \partial_{x_i} \log p_\theta). \]

The proof can be found in Yu et al. (2019). It is easy to verify that given \( g \in \mathcal{G} \), many choices of density functions meet the regularity conditions in Lemma 2.

It worths pointing out that Lemma 1 and 2 are two specifications of the divergence theorem which usually deals with a bounded \( V \). Recently, Mardia et al. studied an SM based on the classic divergence theorem. Barp et al. (2019) proposed a generic version of SM using Stein operators. Chwialkowski et al. (2016); Liu et al. (2016) and a version of divergence theorem which requires weaker conditions (Pigola and Setti, 2014). Other variants of SM also exist, such as replacing the log function with a linear operator (Lyu, 2009). We do not claim (3) to be the most generic version of SM. However, for the purpose of this work, we focus on this specific formulation.

Using Lemma 2, (3) can be written as tractable expectations which does not rely on \( \nabla_x \log q(x) \):

\[ \mathbb{E}_q \| \nabla_x \log p_\theta \circ g \|^2 + 2\mathbb{E}_q \sum_{i=1}^d \partial_{x_i} (g_i^2 \partial_{x_i} \log p_\theta) + C, \]

and this can be further approximated using \( X_q \).

Although this generalized SM only works for densities on \( \mathbb{R}^d_+ \), it is straightforward to modify it so it works for doubly truncated distributions. We can select \( g \) from

\[ \mathcal{G}' := \{ g | g \text{ is conti. diff. and } g(a) = 0, g(b) = 0 \}, \]

to handle distributions that are defined on a product space \( \prod_i [a_i, b_i] \), where \( a_i \) are the \( i \)-th dimension of \( a \). An example of such \( g \) is \( g(x - b) \circ (x - a) \).

However this type of generalized SM cannot deal with arbitrarily bounded domains that cannot be expressed as product spaces, such as a polytope in \( \mathbb{R}^2 \).

It is natural to think that we can similarly design a \( g \) which takes \( 0 \) at the boundary of the truncation domain, so an analogue to Lemma 1 would still give us a tractable form of the estimator. However, we face several issues following this line of reasoning:

- How to construct a computationally efficient \( g \) that would take \( 0 \) at a complex boundary?
- Among all possible choices of \( g \), how to determine which one to use?

Nonetheless, the good news is that we do not need \( g \) to take an analytic form **globally**. The estimator can get by with a function that is easy to evaluate locally and is well defined up to some measure zero domains.

### 4 Trunc-SM

#### 4.1 Objective Function

Suppose \( V \) is a bounded open subspace with a piecewise smooth boundary \( \partial V \). \( \nabla \) denotes the closed subspace \( V \cup \partial V \). Specifically, we require \( V \) to be a Lipschitz domain.

Consider densities defined on \( \mathbb{R}^d \). To estimate the parameter \( \theta \) in \( p_\theta(x) \), we propose the following “maximally weighted SM” objective:

\[ \min_{\theta \in \mathcal{G}} \max_{g \in \mathcal{G}} \mathbb{E}_q(g(x) \cdot \| \nabla_x \log p_\theta(x) - \nabla_x \log q(x) \|_2^2, (5) \]

where \( g : \mathbb{R}^d \rightarrow \mathbb{R} \) and \( \mathcal{G} := \{ g | g(x) = 0, \forall x \in \partial V \} \).

Note this loss takes the geometry of the truncation boundary into consideration through the boundary condition in \( \mathcal{G} \).

The choice of \( g(x) = 0 \) is an analogue to the similar condition in (3).

By using (5), we no longer need to select a specific \( g \). Given a family \( \mathcal{G} \) of functions, it makes sense that we minimize the worst case loss.

Maximizing (5) is infeasible in general. However, it is up to us to choose the family \( \mathcal{G} \) to work in and we show that for Lipschitz continuous functions, we can construct the exact global maximizer of (5).

#### 4.2 Maximizing (5) for Lipschitz Continuous Functions

Let us revise \( \mathcal{G} \) to be

\[ \mathcal{G} := \{ g | g(x) = 0, \forall x \in \partial V \} \]

and \( g \) is \( L \)-Lips. conti., where \( L \) is the Lipschitz constant.

**Proposition 1.**

\[ \max_{g \in \mathcal{G}} \mathbb{E}_q g(x) \cdot \mathcal{L}(x; \theta) = \mathbb{E}_q g_0(x) \cdot \mathcal{L}(x; \theta), \]

where \( g_0(x) := L \cdot \min_{x' \in \partial V} \| x - x' \|, \)
Combining (6) and (7) completes the proof.

Due to the boundary condition of where the last line is due to triangle inequality.

\[
\forall x \in \mathbb{G}, g(x) \leq L \cdot \min_{x' \in \partial V} ||x - x'|| - \min_{x'' \in \partial V} ||x' - x''||
\]
\[
\leq L \cdot \min_{x' \in \partial V} ||x - x'|| - ||x_b - x'||
\]
\[
\leq L \cdot ||x_a - x_b||,
\]

where the last line is due to triangle inequality.

Moreover, \(\forall g \in \mathbb{G}\), we have
\[
g(x) - g(x') = g(x) \leq L||x - x'||, \forall x' \in \partial V
\]
due to the boundary condition of \(\mathbb{G}\) and Lipschitz continuity. Combining (6) and (7) completes the proof.

See Figure 3 for some examples of \(g_0\).

**Proposition 2.** For different choices of Lipschitz constants \(L > 0\), the minimizer of \(g_0\) remains the same.

This is due to the construction of \(g_0\). Changing \(L\) is equivalent as changing the constant that is multiplied to the objective function. The solution to the minimization problem does not change in such cases.

Therefore, we do not need to tune the Lipschitz constant when solving (5).

**4.3 Empirical Approximation of \(E_g g_0(x) \cdot \mathcal{L}(x; \theta)\)**

We have seen the important roles Lemma 1 and 2 play in converting SM objective functions (1) and (3) into tractable expectations.

However, given the construction of \(g_0\), we are presented with a new challenge that \(g_0\) is not a continuously differentiable function (but is continuously differentiable a.e. as we will prove). Classic integration by parts rule on continuously differentiable functions, such as Green’s first identity, Fundamental theorem of calculus, for proving Lemma 1 and 2 cannot be used here. Some extension of integration by parts rule over non-differentiable functions is needed for converting (4) to tractable expectations. First, we state such a theorem from a previous work, Proposition 7.6.1, in Atkinson and Han (2005):

**Theorem 1.** If \(g, f \in H(V)\), where \(H(V)\) is a Sobolev space with order 2 defined on \(V\), then
\[
\int_V \frac{\partial f(x)}{\partial x_i} \cdot g(x) dx := \int_{\partial V} f(x) g(x) n_i - \int_V f(x) \frac{\partial g(x)}{\partial x_i} dx.
\]

where \(\int_V\) is volume integration, \(\int_{\partial V}\) is surface integration on \(\partial V\), \(n_i\) is the normal vector pointing outward from \(\partial V\) and \(n_i\) is the \(i\)-th element of \(n\).

We now want to prove \(g_0 \in H(V)\). By our construction, \(g_0\) is not differentiable on \(V\) globally. However, we can observe that \(g_0\) is continuous and differentiable on \(V\) with exceptions on \(\partial V\) and \(X_c\):

\[
X_c := \left\{ x \in V \big| \text{card} \left[ \text{argmin}_{x' \in \partial V} ||x - x'|| > 1 \right] \right\},
\]

where \(\text{card}(A)\) is the cardinality of a set \(A\). See some examples of \(X_c\) in Figure 3. However, these non-differentiable points occur very rarely on \(g_0\). In fact, \(X_c\) is a measure zero set.

**Proposition 3.** \(X_c\) is a measure zero set.

We provide a sketch proof of this statement in a non-rigorous sense without introducing too many notions in measure theory, for the brevity of the presentation.

**Proof.** Proof by contradiction. \(X_c\) is not a measure zero set, meaning there exists a small \(\epsilon\)-ball in \(\mathbb{R}^d\) where all \(x\) in such a ball are in \(X_c\).

For any \(x_c \in X_c\) and in the \(\epsilon\)-ball, we can pick one of the minimizers \(x_1 \in \text{argmin}_{x' \in \partial V} ||x' - x_c||\). There must exist a point
\( x_m \) which is in the \( \epsilon \)-ball and on the same line between \( x_c \) and \( x_1 \), i.e.
\[
\|x_c - x_m\| + \|x_m - x_1\| = \|x_c - x_1\|. \tag{8}
\]

Since \( x_m \) is in the \( \epsilon \)-ball, we have \( x_m \in X_c \). Then there must exist a point \( x_2 \neq x_1, x_2 \in \partial V \) such that \( \|x_m - x_2\| \leq \|x_m - x_1\| \) due to the definition of \( g_0 \). Combining this inequality with (8), we see
\[
\|x_c - x_2\| \leq \|x_c - x_m\| + \|x_m - x_2\| \leq \|x_c - x_1\|.
\]

The leftmost inequality is due to the triangle inequality and the equality is only attained when \( x_c, x_m, x_2 \) are collinear and \( x_m \) is in between \( x_c \) and \( x_2 \). This together with the fact that \( x_2 \in \partial V \) implying \( x_2 = x_1 \), which cannot happen. So the strict inequality holds:
\[
\|x_c - x_2\| < \|x_c - x_1\|. \tag{9}
\]

This contradicts with the definition of \( x_1 \), being one of the minimizers of \( \min_{x' \in \partial V} \|x' - x_c\| \).

\( \Box \)

See Figure 3 for a visualization of \( \epsilon \)-ball, \( x_1, x_2, x_m \) and \( x_c \) with a triangular \( V \).

**Proposition 4.** \( g_0 \in H(V) \).

**Proof.** Given the measure zero result proved in Proposition 3, a weak derivative can be defined on \( g_0 \) over \( V \). Denote \( x := \arg \min_{x' \in \partial V} \|x' - x\| \). Due to Proposition 3, the weak derivative of \( g_0 \), \( v(x) \in \mathbb{R}^d \) can be uniquely defined as
\[
v(x) := \begin{cases} \frac{x - x_c}{\|x - x_c\|} \cdot L & x \notin X_c \\ \text{arbitrary constant} & x \in X_c \end{cases}
\]

up to a measure zero set \( X_c \).

By our construction of \( v(x) \), \( \|v(x)\|^2 \) is always upper-bounded. Since \( V \) is a bounded domain, we conclude that \( \int_V \|v(x)\|^2 \, dx \leq C \), so \( v(x) \in L^2(V) \).

The existence of a weak derivative which is bounded in \( L^2 \) norm over \( V \) let us conclude that \( g_0 \in H(V) \).

\( \Box \)

**Lemma 3.** If \( \log q(x) \) is continuous differentiable, \( \log p^\theta(x) \) is twice continuously differentiable w.r.t. \( x \), and \( q(x)g_0(x)\partial_x \log p^\theta(x) = 0, \forall x \in \partial V, \forall \theta \),
\[
-E_q(\nabla_x \log p^\theta(x), \nabla_x \log q(x)) \cdot g_0(x) = 0 \quad \text{and} \quad \mathbb{E}_q[\nabla^2_x \log p^\theta(x) \cdot g_0(x)] + \mathbb{E}_q(\nabla_x g_0(x), \nabla_x \log p^\theta(x))
\]

**Proof.** Rewrite
\[
\mathbb{E}_q g_0(x) \cdot (\nabla_x \log p^\theta(x), \nabla_x \log q(x)) = \sum_{i=1}^{d} \int_V \frac{\partial \log p^\theta(x)}{\partial x_i} \cdot \frac{\partial \log q(x)}{\partial x_i} \cdot g_0(x) \, dx, \tag{10}
\]

We can now apply Theorem III on (10) for each \( i \).
\[
\int_V \frac{\partial \log p^\theta(x)}{\partial x_i} \cdot \frac{\partial q(x)}{\partial x_i} \cdot g_0(x) \, dx
\]
\[
= \int_{\partial V} g(x) \cdot \frac{\partial \log p^\theta(x)}{\partial x_i} \cdot g_0(x) n_i - \mathbb{E}_q \frac{\partial [g_0(x) \cdot \nabla_x \log p^\theta(x)]}{\partial x_i}, \tag{11}
\]

The first term in (11) is exactly zero following our assumption. Expanding the second term in (11) and summing over all \( i \) gives the desired result.

This lemma allows us to derive
\[
E_q \mathcal{L}(x; \theta) \cdot g_0(x) = E_q[\log p^\theta(x)] g_0(x) + 2E_q \text{tr} \left[ \nabla^2_x \log p^\theta(x) \right] \cdot g_0(x)
\]
\[
+ 2E_q(\nabla_x g_0(x), \nabla_x \log p^\theta(x)) + C_g, \tag{12}
\]

where \( C_g := E_q[\nabla_x \log q(x)] g_0(x) \). The Trunc-SM minimizes an empirical version of (12) to obtain an estimate of \( \theta \):
\[
\hat{\theta} := \arg \min_{\theta} - \frac{1}{n} \sum_{i=1}^{n} \left[ \nabla_x \log p^\theta(x_i) \right] g_0(x_i)
\]
\[
+ 2 \sum_{i=1}^{n} \text{tr} \left[ \nabla^2_x \log p(x_i; \theta) \right] g_0(x_i)
\]
\[
+ 2 \sum_{i=1}^{n} \langle \nabla_x g_0(x_i), \nabla_x \log p(x_i; \theta) \rangle. \tag{13}
\]

As it was stated in Proposition 3, \( \hat{\theta} \) is the solution for all Lipschitz function families with different Lipschitz constants.

**5 Computation of \( g_0(x) \)**

One of the advantages of choosing such a \( g_0 \) is that \( g_0 \) and its gradient are easy to evaluate given a data point \( x \) and \( \partial V \). For example, if \( \partial V := \{ x \in \mathbb{R}^d | f(x) = 0 \} \), evaluating \( g_0(x) \) can be turned into the following optimization problem:
\[
g_0(x) = \min_{x'} \|x - x'\|, \text{ s.t. } f(x) = 0.
\]

Particularly, if \( \partial V \) consists of multiple line segments defined by \( \langle a_i, x \rangle + b_i = 0 \),
\[
g_0(x) = \min_{i \neq x'} \|x - x'\|, \text{ s.t. } \langle a_i, x \rangle + b_i = 0. \tag{14}
\]

The minimization with respect to \( x' \) is a convex optimization.

The evaluation of \( \nabla_x g_0(x) \) is also straightforward given the projection point \( \hat{x} = \arg \min_{x' \in \partial V} \|x - x'\| \); \( \nabla_x g_0(x) = \frac{x - \hat{x}}{\|x - \hat{x}\|} \) by definition except for \( x \) on \( \partial V \) and \( X_c \) which have measure zero according to Proposition 3.
6 Examples

One criteria of evaluating truncated density model estimator is to see whether it recovers some known sensible estimators when the truncation region expands to \( \mathbb{R}^d \). In this section, we derive the Trunc-SM estimator for a few well-known distributions. We also show some of these Trunc-SM estimators become ordinary MLEs when the truncation region expands to \( \mathbb{R}^d \).

6.1 Truncated Exponential

Exponential distribution itself by definition is on \( \mathbb{R}_+ \). Therefore ordinary SM cannot be used to estimate its parameter. However, using Trunc-SM not only we can derive an estimator for an exponential distribution truncated on \([0, \infty)\), but also recover the MLE as we take \(c \to \infty\).

**Proposition 5.** Let \( p_\lambda(x) := \lambda \exp(-\lambda x) \) truncated on \([0, 2c]\), where \(c > 0\) is a constant, then

\[
\hat{\lambda}(c) := \frac{1}{n} \sum_{i=1}^{n} \frac{\text{sgn}(c - x_i)}{\frac{1}{n} \sum_{i=1}^{n} -|x_i - c| + c}
\]

Moreover, \(\lim_{c \to \infty} \hat{\lambda}(c) = \frac{1}{\sigma} \sum_{i=1}^{n} x_i\), which is the MLE of the non-truncated exponential distribution.

It can be seen that \( g_0(x) = -|c - x| + c \). The derivation of \( \hat{\lambda}(c) \) and its limit immediately follows.

6.2 Two-side Truncated Normal

One-sided truncated normal SM estimator (\( x \in \mathbb{R}_d^+ \)) has been studied in [Hyvärinen, 2007; Yu et al., 2018, 2019]. Here, the two-sided truncated estimator is a simple extension.

**Proposition 6.** Let \( p_\sigma(x) = \mathcal{N}_\sigma(0, \sigma^2) \) be truncated on a domain \([-c, c]\), where \(c > 0\) is a constant:

\[
\hat{\sigma}^2(c) := \frac{1}{n} \sum_{i=1}^{n} \frac{c x_i^2}{c} - \frac{1}{n} \sum_{i=1}^{n} \text{sgn}(x_i) x_i^3
\]

Moreover, \(\lim_{c \to \infty} \hat{\sigma}^2(c) = \frac{1}{n} \sum_{i=1}^{n} x_i^2\) which is the MLE of the variance of an non-truncated, centered normal distribution.

It can be seen that \( g_0(x) = -|x| + c \) and the derivation of \( \hat{\sigma}^2(c) \) and its limit immediately follows.

6.3 Polytope Truncated Normal

Polytope in \( \mathbb{R}^d \) is a generic geometry that can be used to describe the truncation boundary in many scenarios. It is an important special case in terms of computation as the distance of a point \( x \) to the boundary of a polytope can be efficiently formulated as (14).

**Proposition 7.** Let \( p_\mu(x) = \mathcal{N}(\mu, \sigma^2 I_d) \), truncated on \( P \) which is a polytope and \( \sigma \) is known,

\[
\hat{\mu}(c) := \frac{\sum_{i=1}^{n} d_i x_i - \sigma^2 \nabla_x d_i}{\sum_{i=1}^{n} d_i},
\]

where \( d_i = \|x_i - \tilde{x}_i\| \).

Moreover, if \( P \) is a convex polytope defined by

\[
\{ x \in \mathbb{R}^d | A x + b \leq c, A \in \mathbb{R}^{k \times d}, b \in \mathbb{R}^k, c > 0, \}
\]

\[
\lim_{c \to \infty} \hat{\mu}(c) = \frac{1}{n} \sum_{i=1}^{n} x_i\text{, which is the MLE of the mean of an unbounded normal distribution.}
\]

**Proof.** The first statement is easy to see given (13) and the definition of \( g_0 \). We only prove the second statement.

We can normalize each row of \( A \) and rescale \( b, c \) so that all rows in \( A \) has norm 1 and \( P \) remains the same. Then \( d_i \) has a closed form: \( \langle a', x_i \rangle + b - c \), where \( a' \) is a row of \( A \) defines the supporting plane on which the closest projection \( \tilde{x} \) lies. Note for a data point that is inside of the polytope, \( \langle a', x_i \rangle + b - c \) is always negative by definition, so \( d_i = -\langle a', x_i \rangle - b + c \), and \( \nabla_x (\langle a', x_i \rangle - b + c) = -a' \).

Substitute \( d_i \) and \( \nabla_x d_i \) into \( \hat{\mu}(c) \) and divide both numerator and denominator of \( \hat{\mu} \) by \( c \) then take \( c \) to the limit \( \infty \) yields the wanted result. \(\square\)

6.4 Dirichlet on Simplex

Defined on a \( d - 1 \) simplex in \( \mathbb{R}^d \), Dirichlet distribution is often employed as a prior distribution of multinomial distribution. The normalization term is expressed using the Gamma function. However, its parameter estimation given empirical samples is not straightforward. Recent methods use fixed-point iteration to obtain estimates of parameters [Minka, 2012].

We can use Trunc-SM to estimate the parameters of a Dirichlet distribution. However, we must take care of the fact that the gradient \( \nabla_x \log p_\alpha(x) \) and its derivative may not be on the surface of the simplex, so orthogonal projection must be done.

**Proposition 8.** Let \( p_\alpha(x) \propto \exp [(\alpha - 1, \log x)] \) be the Dirichlet distribution defined on a bounded hyperplane in \( \mathbb{R}^d \):

\[
x \in P, P := \{ x \in \mathbb{R}^d | (1, x) = 1 \}.
\]

\[
\alpha = \arg \min_{\alpha} \frac{1}{n} \sum_{i=1}^{n} g_0(x_i) \| T \nabla_x \log p_\alpha(x_i) \|^2 + \frac{2}{n} \sum_{i=1}^{n} g_0(x_i) \sum_{j=1}^{d} \left[ T \nabla_x \nabla_x \log p_\alpha(x_i) \right]_{ij} + \frac{2}{n} \sum_{i=1}^{n} (T \nabla_x \log p_\alpha(x_i), \nabla_x g_0(x_i)),
\]

where \( T \) is the orthogonal projection operator which projects a vector on \( P \): \( Tv := v - \frac{(v, 1)}{d} \) and \( (x, y) \) is the \( j \)-th element of the vector \( x \).
Unfortunately, we cannot establish the relationship between Trunc-SM and MLE in this case. Empirical results also show Trunc-SM is inferior to MLE on non-truncated Dirichlet distributions.

Note the computation of \( g_0 \) can also be formulated as a convex optimization problem as the boundary of a \( d-1 \) simplex consists of \( d \) supporting hyperplanes defined by linear equations \( \langle x, \mu_i \rangle = 1, x_i = 0, \forall i = 1 \ldots d \) and the calculation of \( \nabla x g_0 \) is straightforward after the nearest projection point on the boundary is found. No orthogonal projection is needed for \( \nabla x g_0 \) as it is parallel to \( P \) by definition.

It is in principle possible to estimate density models on truncated manifolds, such as Fisher-von Mises distribution defined on a patch of non-spherical surface. We leave this issue for future investigation.

7 Toy Experiments

We first test our algorithm on randomly generated datasets. We generate samples from a Gaussian mixture on \( \mathbb{R}^2 \), with Gaussian centers at

\[
\mu_1 = [2, 2], \mu_2 = [-2, 2], \mu_3 = [-2, -2], \mu_4 = [2, -2].
\]

The pre-truncated dataset can be seen in Figure 4 as black dots. We limit our observation window to be a green polygon region in the middle, thus only samples are inside the green polygon (blue points in Figure 4) can be observed. The task is to find all four centers of the data generating mixture using only blue points. We generate 10000 samples and only 1417 samples remain after applying such a truncation. The 2D projected visualization of samples can be seen in Figure 5. Our unnormalized model is the unnormalized Dirichlet density: \( p_\alpha(x) \propto \exp((\alpha - 1, \log x)) \).

In this truncated example, \( \partial V \) are three lines defined by intersections of planes:

\[
\begin{align*}
x_1 + x_2 &= 1 \cap x_3 = 0, \\
x_1 + x_3 &= 1 \cap x_2 = 0, \\
x_1 - x_2 &= 0 \cap x_1 + x_2 + x_3 = 1.
\end{align*}
\]

As mentioned, \( g_0 \) can be easily evaluated by solving a convex optimization problem. Estimation results are shown in Figure 5 and it can be seen that Trunc-SM recovers the ground truth reasonably well while the classic MLE, failing to take the truncation region into consideration, gives a skewed estimation.

8 2008 Chicago Crime Dataset

Finally, we test the performance of Trunc-SM on a real-world truncated density estimation problem: We analyse the crime occurrences in Chicago. The dataset contains locations of homicide crimes happened in Chicago during 2008. We fit a Gaussian mixture model with two components on this dataset. The standard derivations of two components are fixed to the same value, which is chosen so that the 80\% percentile radius of an individual Gaussian component can roughly cover the “width” of the city.

The estimated means of two components are plotted in Figure 6. 80\% percentile radius is plotted for the Trunc-SM result. It can be seen, both Trunc-SM and MLE picked the centers at north and south side of the city. The difference however, is at the north site: MLE picked a location inside of the city while the Trunc-SM picked a location right next to the western border of Chicago.

In this case, Trunc-SM tends to put observed crimes on the decaying slope of a Gaussian density which would better explain the sudden truncation of observations at the border and declining rate of crime from the west to the east. MLE, unaware of the truncation, puts the Gaussian center in the middle of the city, while clearly the crimes happen more rarely in the east.
9 Conclusion

We propose an estimator for truncated statistical models with complex truncation boundaries based on a generalized SM. The proposed approach minimizes a maximally weighted SM objective which takes the geometry of the truncation boundary into account. The maximizer $g_0$ among all Lipschitz functions can be easily obtained and evaluated. Moreover, we show such a choice of $g_0$ still allows us to convert an intractable objective function to a tractable objective function. Experiments on toy and Chicago crime dataset show promising results.

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