GBHT: Gradient Boosting Histogram Transform for Density Estimation

Jingyi Cui 1 *  Hanyuan Hang 2 *  Yisen Wang 1  Zhouchen Lin 1 3

Abstract
In this paper, we propose a density estimation algorithm called Gradient Boosting Histogram Transform (GBHT), where we adopt the Negative Log Likelihood as the loss function to make the boosting procedure available for the unsupervised tasks. From a learning theory viewpoint, we first prove fast convergence rates for GBHT with the smoothness assumption that the underlying density function lies in the space $C^{0,\alpha}$. Then when the target density function lies in spaces $C^{1,\alpha}$, we present an upper bound for GBHT which is smaller than the lower bound of its corresponding base learner, in the sense of convergence rates. To the best of our knowledge, we make the first attempt to theoretically explain why boosting can enhance the performance of its base learners for density estimation problems. In experiments, we not only conduct performance comparisons with the widely used KDE, but also apply GBHT to anomaly detection to showcase a further application of GBHT.

1. Introduction
Regarded as one of the most important tasks in unsupervised learning, density estimation aims at inferring the true distribution of targeted unknown variables through limited samples. While basic statistical analysis can be directly carried out on density functions (Scott, 2015), density estimation is further regarded as an imperative cornerstone to more sophisticated tasks, such as anomaly detection (Nachman & Shih, 2020; Zhang et al., 2018; Amarbayasgalan et al., 2018) and clustering (Chen et al., 2020; Parmar et al., 2019; Ghaffari et al., 2019; Jang & Jiang, 2019).

On the other hand, as one of the most successful algorithms over two decades (Bühlmann & Yu, 2003), boosting attracts more and more attention in researches on machine learning (Mathiasen et al., 2019; Cortes et al., 2019; Parnell et al., 2020; Duan et al., 2020; Cai et al., 2020; Suggala et al., 2020). However, when boosting method shows its power and strength in the field of supervised learning, few studies focus on unsupervised learning, especially on the density estimation problem. Furthermore, previous attempts (Ridgeway, 2002; Rosset & Segal, 2003) focus more on methodology study instead of statistical theories. To the best of our knowledge, there remains little understood of the theoretical advantage of boosting over its base learners from the statistical learning point of view.

Under such background, by combing the boosting framework (Rosset & Segal, 2003) with the random histogram transforms (López-Rubio, 2013; Blaser & Fryzlewicz, 2016), this paper aims to establish a new boosting algorithm called Gradient Boosting Histogram Transform (GBHT) for density estimation, which not only has satisfactory performance but also has solid theoretical foundations. To be specific, we adopt the Negative Log Likelihood loss, which makes the boosting method, typically used in supervised learning tasks, available for density estimation which is an unsupervised problem. Moreover, through complete learning theory analysis, we for the first time provide theoretical supports to the benefit of the boosting procedure in the density estimation problem. GBHT starts with generating a random histogram transform consisting of random rotations, stretchings, and translations. (The histogram transforms are i.i.d. generated at each iteration). Then the input space is partitioned into non-overlapping cells corresponding to the unit bin in the transformed space. On those cells, we obtain base learners where piecewise constant functions are applied. Then the iterative process is started with adding a sequence of random histogram transforms for minimizing empirical negative log-likelihood loss by a natural adaption of gradient descent boosting algorithm. Finally, after the iterative process, we inversely transform the partitioned space to the original and obtain the GBHT density estimator.

The contributions of this paper come from the model, theoretical, and experimental perspectives:

- While majority studies of boosting focus on supervised learning, we exploit boosting to improve the accuracy
in density estimation by taking an unsupervised loss function.

- From a learning theory point of view, we prove the fast convergence rates of GBHT with assumptions that the underlying density functions lie in the Hölder space $C^{0,\alpha}$.

- To our best knowledge, we are the first to explain the density estimation problem into a supervised learning problem by rationally adjusting the loss function. Ridgeway (2002) brings EM algorithm in to conduct boosting density estimation. These authors suggest that more researches can be done with boosting for density estimation problems, since present researches about boosting density estimation focus mainly on methodology following the derivation process of gradient descent and none of the above-mentioned boosting works present a satisfactory explanation from the statistical optimization view.

This paper aims at filling the blank in studies of boosting in unsupervised learning, and at providing sound theoretical analysis to explain why boosting can enhance the performance of its base learners for density estimation problems.

3. Methodology

3.1. Notations

Throughout this paper, we assume that $\mathcal{X} \subset \mathbb{R}^d$ is compact and non-empty. For any fixed $r > 0$, we denote $B_r$ as the centered hyper-cube of $\mathbb{R}^d$ with size $2r$, that is, $B_r := [-r, r]^d := \{ x = (x_1, \ldots, x_d) \in \mathbb{R}^d : x_i \in [-r, r], i = 1, \ldots, d \}$, and for any $r' \in (0, r)$, we write $B_{r,r'} := [-r + r', r - r]'^d$. Recall that for $1 \leq p < \infty$, the $L_p$-norm of $x = (x_1, \ldots, x_d)$ is defined by $\|x\|_p := \sqrt[|p|]{\sum_{i=1}^d |x_i|^p}$, and the $L_\infty$-norm is defined by $\|x\|_\infty := \max_{i=1,\ldots,d} |x_i|$.

Throughout this paper, we use the notation $a_n \leq b_n$ and $a_n \geq b_n$ to denote that there exist positive constant $c$ and $c'$ such that $a_n \leq cb_n$ and $a_n \geq c'b_n$, for all $n \in \mathbb{N}$. Moreover, for any $x \in \mathbb{R}$, let $|x|$ denote the largest integer less than or equal to $x$. In the sequel, the following multi-index notations are used frequently. For any vector $x = (x_i)_{i=1}^d \in \mathbb{R}^d$, we write $|x| := (|x_i|)_{i=1}^d$, $x^{-1} := (x_i^{-1})_{i=1}^d$, $\log(x) := (\log x_i)_{i=1}^d$, $\mathcal{F} = \max_{i=1,\ldots,d} x_i$, and $\underline{z} = \min_{i=1,\ldots,d} x_i$.

3.2. Negative Log Likelihood Loss

Let $f$ be the underlying density function of an unknown probability measure $P$ on $\mathcal{X}$. Based on a dataset $D := \{x_1, \ldots, x_n\}$ consisting of i.i.d. observations drawn from $P$, our goal in the density estimation is to construct a measurable function $\hat{f} : \mathcal{X} \rightarrow [0, \infty)$ satisfying $\int_{\mathcal{X}} f(x) \, dx = 1$ to approximate $f$ properly. To evaluate the quality of $\hat{f}$, we use the Negative Log Likelihood loss $L : \mathcal{X} \times [0, \infty) \rightarrow \mathbb{R}$ defined by

$$L(x, \hat{f}) := -\log \hat{f}(x).$$

Then the risk is defined by $\mathcal{R}_{L,P}(\hat{f}) := \int_{\mathcal{X}} L(x, \hat{f}) \, dP(x)$ and the empirical risk is defined by $\mathcal{R}_{L,P}(\hat{f}) := \frac{1}{n} \sum_{i=1}^n L(x_i, \hat{f}(x_i))$. The Bayes rule, which is the smallest possible risk with respect to $P$ and $L$, is given by $\mathcal{R}^*_{L,P} := \inf\{\mathcal{R}_{L,P}(\hat{f}) : \hat{f} : \mathcal{X} \rightarrow \mathbb{R} \}$. In the sequel, the following multi-index notations are used frequently. For any vector $x = (x_i)_{i=1}^d \in \mathbb{R}^d$, we write $|x| := (|x_i|)_{i=1}^d$, $x^{-1} := (x_i^{-1})_{i=1}^d$, $\log(x) := (\log x_i)_{i=1}^d$, $\mathcal{F} = \max_{i=1,\ldots,d} x_i$, and $\underline{z} = \min_{i=1,\ldots,d} x_i$.
We define the histogram transform $H$ to be specific, $R$ denotes the rotation matrix, stretching matrix, and translation vector, respectively.

To be specific, $R$ denotes the rotation matrix which is a real-valued $d \times d$ orthogonal square matrix with unit determinant, that is $R^T = R^{-1}$ and $\det(R) = 1$; $S$ stands for the stretching matrix which is a positive real-valued $d \times d$ diagonal scaling matrix with diagonal elements $(s_i)^d_{i=1}$ that are certain random variables. Obviously, we have $\det(S) = \prod_{i=1}^d s_i$. Moreover, we denote $s = (s_i)^d_{i=1}$, and the bin width vector defined on the input space is given by $h = s^{-1}$. The translation parameter $b \in [0, 1]^d$ is a $d$ dimensional vector named translation vector. Different from rotation and stretching that make no changes to the centroid of data, translation alters the relative position of the transformed data and histogram partition grids. Since we take $h_i' = 1$, where $h_i'$ denotes the bin with of the histogram partition in the transformed space, then if we select $b_i \geq 1$, $i \in [d]$, the same effect can be achieved by using $b_i - 1$. Thus we only need to consider $b_i \in [0, 1]$, i.e. $b \in [0, 1]^d$.

We define the histogram transform $H : \mathcal{X} \to \mathcal{X}$ by

$$H(x) := R \cdot S \cdot x + b.$$  

(2)

Figure 1 illustrates two-dimensional examples of histogram transforms. The left subfigure is the original data and the other two subfigures are possible histogram transforms of the original sample space, with different rotating orientations and scales of stretching.

![Figure 1](image.png)

Figure 1. Two possible histogram transforms in 2-D.

It is important to note that there is no point to consider the bin width $h_i' \neq 1$ in the transformed space, since the same effect can be achieved by scaling the transformation matrix $H'$. Therefore, let $[H(x)]$ be the transformed bin indices, then the transformed bin is $A'_H(x) := \{H'(x') \mid [H'(x')] = [H(x)]\}$ and the corresponding histogram bin containing $x \in \mathcal{X}$ in the input space is $A_H(x) := \{x' \mid H'(x') \in A'_H(x)\}$. Note that here we use $A_H(x)$ and $A'_H(x)$ to denote the cells containing $x$ in the input space and the transformed space, respectively. We further denote all the bins induced by $H$ as $A'_j = \{A_H(x) : x \in \mathcal{X}\}$ with the repetitive bin counted only once, and $\mathcal{I}_H$ as the index set for $H$ such that for $j \in \mathcal{I}_H$, we have $A'_j \cap B_r \neq \emptyset$. As a result, the set $\pi_H := \{A_j\}_{j \in \mathcal{I}_H} := \{A'_j \cap B_r\}_{j \in \mathcal{I}_H}$ forms a partition of $B_r$. For simplicity and uniformity of notations, in the sequel, we denote $\pi_0 = \mathcal{S}_0^{-1}$ and $\pi_0 = \mathcal{S}_0^{-1}$. Then we show a uniform range of $h_i$, denoted as $h_i \in [\pi_0, \pi_0^1]$, for $i = 1, \ldots, d$.

Given a histogram transform $H$, the set $\pi_H = \{A_j\}_{j \in \mathcal{I}_H}$ forms a partition of $B_r$. We consider the following function set $\mathcal{F}_H$ containing piecewise constant density functions

$$\mathcal{F}_H := \left\{ \sum_{j \in \mathcal{I}_H} c_j 1_{A_j} \mid c_j \geq 0, \sum_{j \in \mathcal{I}_H} c_j \mu(A_j) = 1 \right\},$$  

(3)

where $1_{A_j}()$ denotes the indicator function, i.e. $1_{A_j}(x) = 1$ when $x \in A_j$ and 0 otherwise, and $\mu(\cdot)$ is the Lebesgue measure. In order to constrain the complexity of $\mathcal{F}_H$, we penalize on the bin width $h := (h_i)^d_{i=1}$ of the partition $\pi_H$. Then the histogram transform (HT) density estimator can be produced by the regularized empirical risk minimization (RERM) over $\mathcal{F}_H$, i.e.

$$f_{D, H}(h^*) = \arg \min_{f \in \mathcal{F}_H, h \in \mathbb{R}^d} \Omega(h) + \mathcal{R}_{L,D}(f),$$  

(4)

where $\Omega(h) := \lambda h_0^{-2d}$. It is worth pointing out that we adopt the isotropic penalty for each dimension rather than each elements $h_1, \ldots, h_d$ for simplicity of computation.

3.4. Gradient Boosting Histogram Transform (GBHT) for Density Estimation

In this work, we mainly focus on the boosting algorithm equipped with histogram transform density estimators as base learners since they are weak predictors and enjoy computational efficiency. Before we proceed, we need to introduce the function space that we are most interested in to establish our learning theory. Assume that $\{H_j\}_{j=1}^T$ is an i.i.d. sequence of histogram transforms drawn from some probability measure $P_H$ and $\mathcal{F}_t := \mathcal{F}_{H_t}, t = 1, \ldots, T$, are defined as in (3). Then we define the function space $E$ by

$$E := \left\{ f : B_r \to \mathbb{R} \mid f = \sum_{t=1}^T w_t f_t, f_t \in \mathcal{F}_t \text{ s.t. } \sum_{t=1}^T w_t = 1 \right\}.$$  

(5)

As is mentioned above, boosting methods may be viewed as iterative methods for optimizing a convex empirical cost function. To simplify the theoretical analysis, following
the approach of Blanchard et al. (2003), we ignore the dynamics of the optimization procedure and simply consider minimizers of an empirical cost function to establish the oracle inequalities, which leads to the following definition.

**Definition 1** Let $E$ be the function space (5) and $L$ be the negative log-negative loss. Given $\lambda > 0$, we call a learning method that assigns to every $D \in (\mathcal{X} \times \mathcal{Y})^n$ a function $f_{D, \lambda} : \mathcal{X} \to \mathbb{R}$ such that

$$
(f_{D, \lambda}, h^*) = \arg\min_{f \in E, h \in \mathbb{R}^d} \Omega(h) + \mathcal{R}_{L,H}(f)
$$

a gradient boosting histogram transform (GBHT) algorithm for density estimation with respect to $E$, where $\Omega(h) := \lambda h_{\lambda}^{-2d}$.

The regularization term is added to control the bin width of the histogram transform, which has been discussed in Section 3.3. In fact, it is equivalent to adding the $L_\infty$-norm of the base learners $f_t$, since they are piecewise constant functions on the cells with volume no more than $h_{\lambda}^{-d}$.

With all these preparations, we now present the gradient boosting algorithm GBHT to solve the optimization problem (6) in Algorithm 1.

**Algorithm 1** Gradient Boosting Histogram Transform (GBHT) for Density Estimation

**Input:** Training data $D := \{x_1, \ldots, x_n\}$;
Bandwidth parameters $h_{\lambda}, h_0$;
Number of iterations $T$.

**Initialization:** $F_0$ is set to be uniformly distributed on cells $A_j \in \pi_H$ satisfying $A_j \cap D \neq \emptyset$.

for $t = 1 \to T$

Set the sample weight $\omega_{t,i} = 1/F_{t-1}(x_i)$;
For random histogram transformation $H_t$ (2):
Find $f_t^* = \arg\max_{f \in F_t} \sum_{i=1}^n \omega_{t,i} f_t(x_i)$;
Find $\alpha_t := \arg\min_{\alpha} \sum_{i=1}^n -\log \big( (1 + \alpha) F_{t-1}(x_i) + \alpha f_t(x_i) \big)$;
Update $F_t = (1 - \alpha_t) F_{t-1} + \alpha_t f_t$;
end for

**Output:** $F_T$.

The algorithm proceeds iteratively, that is, for $t = 1, \ldots, T$, $F_t(x_i) = (1 - \alpha_t) F_{t-1} + \alpha_t f_t$, where $F_t$ denotes the density estimator after $t$ iterations, $f_t \in F_t$ denotes the $t$-th base learner, and $\alpha_t \in (0, 1)$. Obviously we have $F_t = w_{t,0} F_0 + \sum_{j=1}^t w_{t,j} f_j$, where $w_{t,j} = (1 - \alpha_j) \cdots (1 - \alpha_{j+1}) \alpha_j$ for $j = 1, \ldots, t$, and $w_{t,0} = \prod_{j=1}^t (1 - \alpha_j)$. By initiating $F_0 \in F_0 := H_1$, we have $F_1 \in E$. Then we aim to search the base learner $f_t$ under partition $H_t$ and step size $\alpha_t$ to result in $F_t$ with lower empirical risk $\mathcal{R}_{L,H}(F_t)$ in each iteration. In the $t$-th iteration, for every $\alpha_t \in (0, 1)$, the minimization of $\mathcal{R}_{L,H}(F_t)$ equals to the minimization of $\sum_{i=1}^n -\log(F_{t-1}(x_i) + \epsilon_t f_t(x_i))$, where $\epsilon_t = \alpha_t/(1 - \alpha_t)$. Using Taylor expansion, we get

$$
\sum_{i=1}^n -\log(F_{t-1}(x_i) + \epsilon_t f_t(x_i)) = \sum_{i=1}^n -\log(F_{t-1}(x_i)) - \epsilon_t \cdot \omega_{t,i} f_t(x_i) + O(\epsilon_t^2),
$$

where $\omega_{t,i} := 1/F_{t-1}(x_i)$. For sufficiently small $\epsilon_t$ (or $\alpha_t$), we can ignore the higher order term and find the maximum gradient $\max_{f_t \in F_t} \sum_{i=1}^n \omega_{t,i} f_t(x_i)$. Then we determine the step size $\alpha_t$ by line search, which ensures that the updated $F_t$ remains to be a probability distribution.

It is worth mentioning that GBHT enjoys two advantages. First, the algorithm can be locally adaptive by applying random rotations, stretchings, and translations to the original input data. Regular density estimators such as KDE adopt uniform bandwidth, regardless of the fact that the local structures of real-world data usually vary from area to area. On the contrary, it is well known that boosting algorithms take local data structures into consideration by updating its vulnerable part in each iteration, and the adopted histogram transform catches exactly various local features of the input data. Thus, good combinations of random weak learners and the boosting procedure can lead to great local adaptivity. Second, the boosting procedure brings smoothness to histogram-based density estimators, thanks to the randomness of base learners. Through iteration, GBHT adds more information obtained by the base learners into the boosting estimator, and it turns out to be the weighted average of all random base learners with different partition boundaries. As a result, it can be more smooth than regular histogram density estimators, which will also be theoretically verified in Section 4 and experimentally validated by numerical simulations in Section 5.3.

**4. Theoretical Results**

Our theoretical analysis is built on the fundamental assumption on the smoothness of the underlying density function. Recall that a function $f : \mathcal{X} \to \mathbb{R}$ is $(k, \alpha)$-Hölder continuous, $\alpha \in (0, 1]$, $k \in \mathbb{N}_0$, if there exists a constant $c_L \in (0, \infty)$ such that

$$
\|\nabla^\ell f\| \leq c_L \text{ for all } \ell \in \{1, \ldots, k\} \quad (7)
$$

$$
\|\nabla^k f(x) - \nabla^k f(x')\| \leq c_L \|x - x'|^\alpha \quad (8)
$$

for all $x, x' \in B_r$. The set of such functions is denoted by $C^{k,\alpha}(B_r)$. Note that the functions contained in the space $C^{k,\alpha}$ with larger $k$ enjoy a higher level of smoothness. Throughout this paper, we make the following assumptions on the bin width $h$. 

Assumption 1 Let the bin width \( h \in [h_0, \bar{h}_0] \) and assume that there exists some constant \( c_0 \in (0, 1) \) such that \( c_0 \bar{h}_0 \leq h_0 \leq c_0^{-1} \bar{h}_0 \). Moreover, if the bin width \( h \) depends on the sample size \( n \), that is, \( h_n \in [h_{0,n}, \bar{h}_{0,n}] \), we still have \( c_0 \bar{h}_{0,n} \leq h_{0,n} \leq c_0^{-1} \bar{h}_{0,n} \).

Assumption 1 indicates that the upper and lower bounds of the bin width \( h \) are of the same order. In other words, we assume that under a certain partition, the extent of stretching in each dimension cannot vary too much.

Furthermore, to remove the boundary effect on the convergence rate, we denote \( L_{\pi_0}(x, t) \) as the negative log loss function restricted to \( B^+_R(x, \pi_0) \), that is,
\[
L_{\pi_0}(x, t) := 1_{B^+_R(x, \pi_0)}(x)L(x, t),
\]
where \( L(x, t) \) is the negative log loss.

4.1. Convergence Rates for GBHT in \( C^{0, \alpha} \)

Theorem 1 Let \( f_{D, \lambda} \) be as in (6) and the density function \( f \in C^{0, \alpha}(B_r) \). Then for all \( \tau > 0 \) and for any \( \delta \in (0, 1) \), there exists a constant \( N_0 \) such that for all \( n \geq N_0 \), there holds
\[
\mathcal{R}_{L, P}(f_{D, \lambda}) - \mathcal{R}_{L, P}^* \lesssim n^{-\frac{2(1+\alpha)}{(4+2\delta)(1+\alpha)/(1+\alpha)+d}},
\]
with probability \( P^n \otimes P_H \) at least \( 1 - 3e^{-\tau} \).

Theorem 1 presents the fast convergence rates of the GBHT density estimator in the sense of “with high probability”, which is a stronger claim than the convergence results “in expectation”. Moreover, convergence rates, a finite sample property of GBHT, also indicate the consistency of our GBHT attains asymptotically convergence rate which is slightly faster than \( n^{-2(1+\alpha)/(4(1+\alpha)+d)} \).

4.2. Convergence Rates for GBHT in \( C^{1, \alpha} \)

Theorem 2 Let \( f_{D, \lambda} \) be as in (6) and the density function \( f \in C^{1, \alpha}(B_r) \). Moreover, let \( L_{\pi_0}(x, t) \) be the restricted negative log loss as in (9). Then for all \( \tau > 0 \) and \( \delta \in (0, 1) \), there exists a constant \( N_1 \) such that for all \( n \geq N_1 \), by choosing \( T_n \gtrsim n^{2\alpha/(2(1+\alpha)(2-\delta)+d)} \), there holds
\[
\mathcal{R}_{L_{\pi_0}, P}(f_{D, \lambda}) - \mathcal{R}^*_{L_{\pi_0}, P} \lesssim n^{-\frac{2(1+\alpha)}{(2+\alpha)(2-\delta)+d}},
\]
with probability \( P^n \otimes P_H \) not less than \( 1 - 4e^{-\tau} \) in expectation with respect to \( P_H \).

In Theorem 2, the excess risk decreases as \( T_n \) grows at first, and when \( T_n \) achieves a certain level, the algorithm achieves the best convergence rate. Moreover, comparing with Theorem 1, when the underlying density function turns more smooth, GBHT achieves a better convergence rate with \( f \in C^{1, \alpha}(B_r) \) than that with \( f \in C^{0, \alpha}(B_r) \), where a relatively large \( T_n \) helps the density estimator to achieve asymptotic smoothness.

4.3. Lower Bound for HT Density Estimation in \( C^{1, \alpha} \)

Theorem 3 Let \( f_{D, H} \) be as in (4) and suppose that the density function \( f \in C^{1, \alpha}(B_r) \). Then there exists a constant \( N_2 \) such that for all \( n \geq N_2 \), there holds
\[
\sup_{f \in C^{1, \alpha}} \mathcal{R}_{L, P}(f_{D, H}) - \mathcal{R}^*_{L, P} \gtrsim n^{-\frac{2\alpha}{(2+\alpha)(2-\delta)+d}},
\]
in expectation with respect to \( P^n \otimes P_H \).

Recall that in Theorem 2, as \( n \to \infty \), the upper bound for our GBHT attains asymptotically convergence rate which is smaller than \( n^{-2(1+\alpha)/(4(1+\alpha)+d)} \). When comparing Theorem 3 with Theorem 2, we find that for any \( \alpha \in (0, 1] \), and \( d \gtrsim 2(1+\alpha) \), the upper bound of the convergence rate (10) for GBHT turns out to be smaller than the lower bound (11) for HT density estimators, which explains the benefits of the boosting procedure from the perspective of convergence rates.

5. Numerical Experiments

5.1. Generation Methods of Histogram Transforms

Here we describe a practical method for the construction of histogram transforms we are confined to in this study. Starting with a \( d \times d \) square matrix \( M \), consisting of \( d^2 \) independent univariate standard normal random variates, a Householder QR decomposition is applied to obtain a factorization of the form \( M = R \cdot W \), with an orthogonal matrix \( R \) and an upper triangular matrix \( W \) with positive diagonal elements. The resulting matrix \( R \) is orthogonal by construction and can be shown to be uniformly distributed. Unfortunately, if \( R \) does not feature a positive determinant then it is not a proper rotation matrix according to the definition of \( R \). In this case, we can change the sign of the first column of \( R \) to construct a new rotation matrix \( R^+ \).

We apply the well-known Jeffreys prior for scale parameters (Jeffreys, 1946). To be specific, we draw \( \log(s_i) \) from the uniform distribution over intervals \([\log(h_0), \log(\bar{h}_0)]\). Recall that \( h = s^{-1} \) stands for the bin width vector measured in the input space, we choose \( h_0 \) and \( \bar{h}_0 \), recommended by (López-Rubio, 2013), as \( \bar{h} = 3.5s^{-1/2} \), where
We base the simulations on four different types of synthetic distributions, each with dimension \(d \in \{2, 5, 7\}\), respectively. The premise of constructing data sets is that we assume that the components \(X_i \sim f_i\), \(i = 1 \ldots d\), of the random vector \(X = (X_1, \ldots, X_d)\) are independent of each other. To be specific, Type I density function, representing a bimodal Gaussian distribution, enjoys high order of smoothness, while those for Types II and III are not continuous. Moreover, Types II and III represent density functions with bounded support and unbounded support, respectively. Finally, Type IV represents the case where the marginal distributions of each dimension are not identical. More detailed descriptions and visual illustrations are shown in Section C.1 of the supplementary material.

In the following experiments, we generate 2,000 and 10,000 i.i.d samples as training and testing data respectively from each type of synthetic datasets, and each with dimension \(d \in \{2, 5, 7\}\).

5.3.2. The Power of Boosting

To show the behavior of \(T\), we carry out the experiments with \(T \in \{1, 5, 10, 20, 50, 100, 500, 1000\}\), and the other two hyper-parameters are chosen by 3-fold cross-validation. We pick \(s_{\min}\) from the set \{-3 + 0.5k, k = 0, \ldots, 12\} and \(s_{\max} - s_{\min}\) is chosen from the set \{0.5 + 0.5k, k = 0, \ldots, 5\}. For each \(T\) we repeat this procedure for 10 times.

Figure 2. The study of parameter \(T\) on GBHT of Type I synthetic distribution, where the first row illustrates the low-dimensional results with dimension \(d = 2\), and the second row indicates the high-dimensional results with dimension \(d = 5\). The left column indicates how \(MAE\) varies along parameters \(T\), and the right column shows the variation of \(ANLL\).

As can be seen in Figure 2, as \(T\) grows, the accuracy performance of GBHT (both \(MAE\) and \(ANLL\)) first enhances dramatically when \(T\) grows from 1 to 1,000, but as \(T\) continues to grow, a steady state will be reached. This coincides with Theorem 2, where the convergence rate attains the optimum when \(T_n\) is greater than a certain value. Moreover, fewer iterations are required to make GBHT convergence when the dimension of input space is lower. A large number of iterations lead to a more accurate model but bring about the additional burden of computation.

For a possible explanation of the enhancement in estimation accuracy under the boosting procedure, we conduct simulations to show that GBHT achieves asymptotic smoothness with \(T\) increasing. For the sake of more clear visualization, we utilize a toy example with 2,000 samples i.i.d. generated from the one-dimensional standard normal distribution, and
use GBHT to conduct density estimation, where the number of trees $T$ is set to 1, 5, 20, 50, respectively.

![Figure 3](image1)

**Figure 3.** The study of parameter $T$ on GBHT of the Standard Normal distribution. The red line represents the underlying density while the blue one represents density estimator returned by GBHT.

From Figure 3 we see that with $T = 1$, the base estimator turns out to be a step function with discontinuous boundaries, and the estimation is far from satisfactory. Nevertheless, as the iteration $T$ increases, the boosting estimator becomes more continuous and smooth with the corresponding accuracy enhancing greatly. With $T = 50$, our GBHT is nearly smooth and achieves high estimation accuracy.

### 5.3.3. Parameter Analysis

Here we mainly conduct experiments concerning the parameters of histogram transforms, namely the lower and upper scale parameters $s_{\text{min}}, s_{\text{max}} \in \mathbb{R}$. To this end, for the sake of clear visualization, we consider the Type I synthetic dataset of 1 dimension to see how these parameters affect the performance of GBHT.

Recall that the scale parameters $s_{\text{min}}$ and $s_{\text{max}}$ of the stretching matrix $S$ control the size of histogram bins. Smaller bins are required for the regions with complex structures of the density function while those with simple structure calls for larger bins. A narrower range of bin size is accommodated to cope with the varying scales while preserving a homogeneous structure. We conduct experiments over four pairs of scale parameters $(s_{\text{min}}, s_{\text{max}}) \in \{(-2.5, -1.5), (-2, -1), (-1.5, -0.5), (-1, 0)\}$. We select $T = 500$ to make the density estimator convergence with sufficient boosting iterations.

As is shown in Figure 4, lower values of these parameters (larger bin width) lead to a coarser approximation of the underlying density function, which results in the loss of precision. Figure 4(a) implies that the density estimator is underfitting when the bin width is too large. On the contrary, if the bin width is too small, then there are few samples lying in most of the histogram bins and thus overfitting occurs as shown in Figure 4(d). Therefore, it is of great importance to choose $s_{\text{min}}$ and $s_{\text{max}}$ properly.

![Figure 4](image2)

**Figure 4.** The study of parameter $s_{\text{min}}$ and $s_{\text{max}}$ on GBHT of the Type I synthetic distribution. The red line represents the density estimator returned by GBHT algorithm while the blue one represents the underlying density function. And the tuples in subtitle represent $(s_{\text{min}}, s_{\text{max}})$.

### 5.4. Performance Comparisons

In this section, we conduct performance comparisons on both synthetic and real datasets. Recall that both our theoretical results (shown in Theorems 2 and 3) and empirical illustrations (shown in Figure 3) demonstrate that boosting improves the performance of histogram-based methods by enhancing the smoothness of the estimator. Therefore, we compare our GBHT with the kernel density estimator (KDE) which enjoys high order of smoothness. We also compare our GBHT with MIX (Ridgeway, 2002), a boosting method for density estimation using mixtures. We also consider the histogram density estimator (HDE), which can be viewed as a special case of our GBHT when $T = 1$ and $H = I$ (identity matrix). We run HDE on synthetic datasets with the bin width chosen by Sturges’ rule (Sturges, 1926).

### 5.4.1. Synthetic Data Comparisons

Following the experimental settings in Section 5.3, we conduct empirical comparisons between GBHT and the prevailing KDE to further demonstrate the desirable performance of GBHT under synthetic datasets. Table 1 records average $\text{ANLL}$ and $\text{MAE}$ over simulation data sets for KDE and GBHT with $T = 1, 000$. For higher dimensions $d = 5$ and $d = 7$, our GBHT always outperforms KDE in terms of...
5.4.2. Real Data Comparisons

We conduct real data comparisons on real datasets from the UCI repository. We put the detailed description of datasets in Section C.2 of the supplement.

**Experimental Settings.** In order to evaluate the performance of density estimators on datasets with various dimensions, we apply the following data preprocessing pipeline. Firstly, we remove duplicate observations as well as those with missing values. Then each dimension of the datasets is scaled to [0, 1] and each dataset is reduced to lower dimensions $d'$ through PCA, e.g. to 10%, 30%, 50% and 70% of the original dimension $d$, respectively. Finally, in each dataset, we randomly select 70% of the samples for training and the remaining 30% for testing.

The number of iterations $T$ is set to 100 and the other two hyper-parameters $s_{\min}$ and $s_{\max} - s_{\min}$ are chosen from $\{-2 + 0.5k, k = 0, \ldots, 8\}$ and $\{0.5 + 0.5k, k = 0, \ldots, 5\}$, respectively, by 3-fold cross-validation. We repeat this procedure 10 times to evaluate the standard deviation for ANLL. The average ANLL on test sets are recorded in Table 2.

Since real density often resides in a low-dimensional manifold instead of filling the whole high-dimensional space, it is reasonable to study the density estimation problem after dimensionality reduction. Therefore, in data preprocessing, all data sets are reduced to various lower dimensions through PCA. However, we need to take the to-be-reduced dimension as a hyper-parameter, since in general, the dimension of the manifold is unknown.

**Experimental Results.** In Table 2, we summarize the comparisons with the state-of-the-art density estimator KDE on six real datasets, which demonstrates the accuracy of our GBHT algorithm. For most of the redacted datasets, GBHT shows its superiority on accuracy, whereas the standard deviation of GBHT is slightly larger than that of KDE due to the randomness of histogram transforms.

### 5.5. Gradient Boosted Histogram Transform (GBHT) for Anomaly Detection

To showcase a potential application of GBHT, we propose a density-based method for anomaly detection. Given a density level $\rho$, we regard the sample points with low density estimation $\{x_i \in D \mid f_{D,\lambda}(x_i) \leq \rho\}$ as anomaly points. Based on GBHT density estimation, we are able to present the Gradient Boosting Histogram Transform (GBHT) for anomaly detection in Algorithm 2.

**Algorithm 2 GBHT for Anomaly Detection**

**Input:** Training data $D := \{x_1, \ldots, x_n\}$; Density threshold parameters $\rho$.

Compute GBHT $f_{D,\lambda} (6)$.

**Output:** Recognize anomalies as

$$\{x_i \in D \mid f_{D,\lambda}(x_i) \leq \rho\}.$$

We conduct numerical experiments to make a comparison between our GBHT and several popular anomaly detection algorithms such as the forest-based Isolation Forest (iForest) (Liu et al., 2008), the distance-based $k$-Nearest Neighbor ($k$-NN) (Ramaswamy et al., 2000) and Local Outlier Factor (LOF) (Breunig et al., 2000), and the kernel-based one-class SVM (OCSVM) (Schölkopf et al., 2001), on 20 real-world benchmark outlier detection datasets from the ODDS library. We perform ranking according to the best AUC performance when parameters go through their parameter grids. Detailed experimental settings and comparison results are shown in Section C.3.

In the aspect of best performance, our method GBHT wins in 7 out of 20 datasets, while the iForest and OCSVM win both 4 out of 20 datasets, respectively. Moreover, our GBHT ranks the second on 5 datasets. Finally, in the aspect of the average performance of benchmark datasets, our method

**Table 1. Average ANLL and MAE over simulated datasets**

| $d$ | Method       | Type I |       | Type II |       | Type III |       | Type IV |       |
|-----|--------------|--------|-------|---------|-------|----------|-------|---------|-------|
|     |              | ANLL   | MAE   | ANLL    | MAE   | ANLL     | MAE   | ANLL    | MAE   |
| 5   | GBHT (Ours)  | 6.26   | 2.41e-3 | -0.80  | 10.31 | 8.23     | 6.61e-4 | 3.85   | 0.14  |
|     | KDE          | 6.33   | 2.36e-3 | -0.32  | 12.40 | 8.65     | 8.27e-4 | 3.86   | 0.15  |
|     | MIX          | 6.53   | 3.08e-3 | 1.82   | 13.91 | 9.64     | 9.54e-4 | 5.35   | 0.14  |
|     | HDE          | 9.33   | 4.86e-3 | 10.17  | 19.70 | 10.77    | 1.33e-3 | 6.09   | 0.17  |
| 7   | GBHT (Ours)  | 8.36   | 4.33e-4 | -0.45  | 34.91 | 10.81    | 5.30e-5 | 5.10   | 0.18  |
|     | KDE          | 8.77   | 5.13e-4 | 0.03   | 40.74 | 12.48    | 6.05e-5 | 5.16   | 0.18  |
|     | MIX          | 8.65   | 5.38e-4 | 2.61   | 42.13 | 11.34    | 6.32e-5 | 7.02   | 0.19  |
|     | HDE          | 11.35  | 1.45e-3 | 11.48  | 73.97 | 11.49    | 1.05e-4 | 9.88   | 0.20  |

* The best results are marked in **bold**.
GBHT: Gradient Boosting Histogram Transform for Density Estimation

Table 2. Average ANLL over real data sets

| Datasets   | d’  | GBHT | KDE | MIX | Datasets   | d’  | GBHT | KDE | MIX |
|------------|-----|------|-----|-----|------------|-----|------|-----|-----|
| Adult      | 2   | -1.2371 | -0.7402 | 1.3572 | Diabetic    | 1   | -0.7057 | -0.2627 | 0.7131 |
|            |     | (0.0312) | (0.0027) | (0.0050) |            |     | (0.1253) | (0.0111) | (0.0186) |
|            | 4   | -1.9312 | -0.3075 | 1.7609 |            | 3   | -1.5982 | -0.4042 | 0.5193 |
|            |     | (0.0667) | (0.0032) | (0.0059) |            |     | (0.1011) | (0.0403) | (0.0600) |
|            | 8   | -5.5922 | -2.2970 | 0.8562 |            | 4   | -1.8605 | -0.8353 | 0.0403 |
|            |     | (0.1097) | (0.0108) | (0.3183) |            |     | (0.1424) | (0.0773) | (0.0771) |
|            | 10  | -6.0740 | -3.4372 | -0.8975 |            | 6   | -2.6134 | -1.9693 | -1.2393 |
|            |     | (0.1044) | (0.0110) | (0.0982) |            |     | (0.2310) | (0.1550) | (0.1087) |
|           |     |       |       |       | Australian | 2   | -0.7966 | 1.3155 | 1.8577 |
|            |     | (0.0904) | (0.0234) | (0.0263) |            |     | (0.0917) | (0.0423) | (0.0776) |
|            | 4   | -5.8510 | 0.8518 | 3.0147 |            | 10  | 4.1625 | 4.6447 | 1.3366 |
|            |     | (0.2947) | (0.0291) | (0.0370) |            |     | (0.2150) | (0.4448) | -         |
|            | 8   | -3.7957 | 0.6879 | 2.6446 |            | 17  | 3.8920 | 5.3236 | 1.3366 |
|            |     | (0.5823) | (0.1056) | (0.6659) |            |     | (0.4198) | (0.9654) | -         |
|            | 10  | -1.3659 | 0.4995 | 2.2421 |            | 24  | 2.1412 | 4.5570 | 1.3366 |
|            |     | (0.4382) | (0.1748) | (0.4280) |            |     | (0.6710) | (1.3684) | -         |
| Breast-cancer | 1   | 0.3580 | 0.6907 | 1.3141 | Parkinsons | 2   | 0.9465 | 0.0847 | 1.0913 |
|            |     | (0.0561) | (0.0394) | (0.0246) |            |     | (0.0402) | (0.0094) | (0.0172) |
|            | 3   | -0.5446 | 0.1743 | 0.7889 |            | 7   | 5.7700 | 2.1513 | 0.1867 |
|            |     | (0.1887) | (0.1268) | (0.0626) |            |     | (0.1439) | (0.0189) | (0.0538) |
|            | 6   | -3.2099 | -1.1379 | -0.7526 |            | 10  | 10.0932 | 7.8291 | 5.6844 |
|            |     | (0.6068) | (0.2788) | (0.4959) |            |     | (0.1492) | (0.0340) | (0.0906) |
|            | 8   | -6.4362 | -2.1110 | -3.1482 |            | 11  | 16.9316 | -16.8767 | -15.6404 |
|            |     | (0.8144) | (0.3906) | (0.6501) |            |     | (0.2151) | (0.1025) | (0.1163) |

* The best results are marked in bold, and the standard deviation is reported in the parenthesis. The results of MIX on Ionosphere with d’ = 10, 17, 24 is corrupted due to numerical problems.

has the lowest rank-sum. Overall, our experiments on benchmark datasets show that our method has favorable performance among competitive anomaly detection algorithms.

6. Conclusion

In this paper, we propose an algorithm called Gradient Boosting Histogram Transform (GBHT) for density estimation with novel theoretical analysis under the RERM framework. It is well-known that boosting methods are hard to apply in unsupervised learning. Therefore, we turn the density estimation into a supervised learning problem by changing the loss function to Negative Log Likelihood loss, which measures the proximity between the estimated density and the true one. In each iteration of boosting methods, histogram transform first randomly stretches, rotates, and translates the feature space for acquiring more information, and then an additional density function is attached to the estimated one with weights, which guarantees that the result is a density function with integral equals to 1. For theoretical achievements, we prove the convergence properties of our algorithm under mild assumptions. It should be highlighted that we are the first to explain the benefits of the boosting procedure for density estimation algorithms. Last but not least, numerical experiments of both synthetic data and real data are carried out to verify the promising performance of GBHT with applications to anomaly detection.

Acknowledgement

Yisen Wang is supported by the National Natural Science Foundation of China under Grant No. 6206153, CCF-Baidu Open Fund (No. OF2020002), and Project 2020BD006 supported by PKU-Baidu Fund. Zhouchen Lin is supported by the National Natural Science Foundation of China (Grant No.s 61625301 and 61731018), Project 2020BD006 supported by PKU-Baidu Fund, Major Scientific Research Project of Zhejiang Lab (Grant No.s 2019KB0AC01 and 2019KB0AB02), and Beijing Academy of Artificial Intelligence.

References

Amarbayasgalan, T., Jargalsaikhan, B., and Ryu, K. H. Unsupervised novelty detection using deep autoencoders with density based clustering. *Applied Sciences, 8*(9):
GBHT: Gradient Boosting Histogram Transform for Density Estimation

1468, 2018.

Biau, G., Cadre, B., and Rouvière, L. Accelerated gradient boosting. *Machine Learning*, 108(6):971–992, 2019.

Blanchard, G., Lugosi, G., and Vayatis, N. On the rate of convergence of regularized boosting classifiers. *The Journal of Machine Learning Research*, 4(Oct):861–894, 2003.

Blaser, R. and Fryzlewicz, P. Random rotation ensembles. *The Journal of Machine Learning Research*, 17(1):126–151, 2016.

Breiman, L. Some infinity theory for predictor ensembles. Technical report, Technical Report 579, Statistics Dept. UCB, 2000.

Breunig, M. M., Kriegel, H.-P., Ng, R. T., and Sander, J. Lof: identifying density-based local outliers. In *ACM Sigmod Record*, volume 29, pp. 93–104. ACM, 2000.

Bühlmann, P. and Yu, B. Boosting with the L2 loss: regression and classification. *Journal of the American Statistical Association*, 98(462):324–339, 2003.

Cai, Y., Hang, H., Yang, H., and Lin, Z. Boosted histogram transform for regression. In *International Conference on Machine Learning*, pp. 1251–1261. PMLR, 2020.

Chen, T. and Guestrin, C. Xgboost: A scalable tree boosting system. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pp. 785–794, 2016.

Chen, Y., Hu, X., Fan, W., Shen, L., Zhang, Z., Liu, X., Du, J., Li, H., Chen, Y., and Li, H. Fast density peak clustering for large scale data based on knn. *Knowledge-Based Systems*, 187:104824, 2020.

Cortes, C., Mohri, M., and Storcheus, D. Regularized gradient boosting. *Advances in Neural Information Processing Systems*, 32:5449–5458, 2019.

Criminisi, A. and Shotton, J. *Decision Forests for Computer Vision and Medical Image Analysis*. Springer Science & Business Media, 2013.

Criminisi, A., Shotton, J., and Konukoglu, E. Decision forests for classification, regression, density estimation, manifold learning and semi-supervised learning. *Microsoft Research Technical Report 2011–114*, 2011.

Duan, T., Anand, A., Ding, D. Y., Thai, K. K., Basu, S., Ng, A., and Schuler, A. Ngboost: Natural gradient boosting for probabilistic prediction. In *International Conference on Machine Learning*, pp. 2690–2700. PMLR, 2020.

Freund, Y. and Schapire, R. E. A decision-theoretic generalization of on-line learning and an application to boosting. *Journal of Computer and System Sciences*, 55(1):119–139, 1997.

Friedman, J. H. Greedy function approximation: a gradient boosting machine. *The Annals of Statistics*, pp. 1189–1232, 2001.

Ghaffari, M., Lattanzi, S., and Mitrović, S. Improved parallel algorithms for density-based network clustering. In *International Conference on Machine Learning*, pp. 2201–2210. PMLR, 2019.

Jang, J. and Jiang, H. DBSCAN++: Towards fast and scalable density clustering. In *International Conference on Machine Learning*, pp. 3019–3029. PMLR, 2019.

Jeffreys, H. An invariant form for the prior probability in estimation problems. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, 186(1007):453–461, 1946.

Klemelä, J. Multivariate histograms with data-dependent partitions. *Statistica Sinica*, 19(1):159–176, 2009.

Liu, F. T., Ting, K. M., and Zhou, Z.-H. Isolation forest. In *Proceedings of the IEEE International Conference on Data Mining*, pp. 413–422, 2008.

Liu, L. and Wong, W. H. Multivariate density estimation via adaptive partitioning (I): sieve MLE. *arXiv preprint arXiv:1401.2597*, 2014.

López-Rubio, E. A histogram transform for probability density function estimation. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 36(4):644–656, 2013.

Mathiasen, A., Larsen, K. G., and Grønlund, A. Optimal minimal margin maximization with boosting. In *International Conference on Machine Learning*, pp. 4392–4401. PMLR, 2019.

Nachman, B. and Shih, D. Anomaly detection with density estimation. *Physical Review D*, 101(7):075042, 2020.

Parmar, M., Wang, D., Zhang, X., Tan, A.-H., Miao, C., Jiang, J., and Zhou, Y. Redpc: A residual error-based density peak clustering algorithm. *Neurocomputing*, 348:82–96, 2019.

Parnell, T., Anghel, A., Łazuka, M., Ioannou, N., Kurella, S., Agarwal, P., Papandreou, N., and Pozidis, H. Snapboost: A heterogeneous boosting machine. *Advances in Neural Information Processing Systems*, 33, 2020.

Ram, P. and Gray, A. G. Density estimation trees. In *Proceedings of the 17th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pp. 627–635. ACM, 2011.
Ramaswamy, S., Rastogi, R., and Shim, K. Efficient algorithms for mining outliers from large data sets. In *Proceedings of the ACM SIGMOD International Conference on Management of Data*, pp. 427–438, 2000.

Ridgeway, G. Looking for lumps: Boosting and bagging for density estimation. *Computational Statistics & Data Analysis*, 38(4):379–392, 2002.

Rosset, S. and Segal, E. Boosting density estimation. In *Advances in Neural Information Processing Systems*, pp. 657–664, 2003.

Schapire, R. and Freund, Y. A decision-theoretic generalization of on-line learning and an application to boosting. In *Second European Conference on Computational Learning Theory*, pp. 23–37, 1995.

Schölkopf, B., Platt, J. C., Shawe-Taylor, J., Smola, A. J., and Williamson, R. C. Estimating the support of a high-dimensional distribution. *Neural Computation*, 13(7): 1443–1471, 2001.

Scott, D. W. *Multivariate Density Estimation*. John Wiley & Sons, Inc., Hoboken, NJ, second edition, 2015.

Steinwart, I. and Christmann, A. *Support Vector Machines*. Information Science and Statistics. Springer, New York, 2008.

Sturges, H. A. The choice of a class interval. *Journal of the American Statistical Association*, 21(153):65–66, 1926.

Suggala, A., Liu, B., and Ravikumar, P. Generalized boosting. *Advances in Neural Information Processing Systems*, 33, 2020.

Van der Vaart, A. W. and Wellner, J. A. *Weak Convergence and Empirical Processes*. Springer Series in Statistics. Springer-Verlag, New York, 1996.

Vapnik, V. N. and Chervonenkis, A. Y. On the uniform convergence of relative frequencies of events to their probabilities. In *Measures of Complexity*, pp. 11–30. Springer, 2015.

Zhang, L., Lin, J., and Karim, R. Adaptive kernel density-based anomaly detection for nonlinear systems. *Knowledge-Based Systems*, 139:50–63, 2018.
Appendix

This file consists of supplementaries for both theoretical analysis and experiments. In Section A, we divide the general risk into approximation error and estimation error term for the underlying density function residing in space $C^{0,\alpha}$ and $C^{1,\alpha}$, respectively. The corresponding proofs of Section A and Section 4 are shown in Section B. In Section C we show the supplementaries for numerical experiments.

A. Error Analysis

This section provides a more comprehensive error analysis for the theoretical results in Section 4. To be specific, we conduct approximation error analysis for the boosted density estimators $f_{D, \lambda}$ under the assumption that the density function $f_{L, \lambda}$ lying in the Hölder spaces $C^{0,\alpha}$ and $C^{1,\alpha}$.

To conduct the theoretical analysis, we also need the infinite sample version of Definition 1. To this end, we fix a distribution $P$ on $X$ and the function space $E$ be as in (5). Then every $f_{L, \lambda} \in E$ satisfying

$$\Omega(h) + R_{L, \lambda}(f_{L, \lambda}) = \inf_{f \in E} \Omega(h) + R_{L, \lambda}(f)$$

is called an infinite sample version of GBHT with respect to $E$ and $L$. Moreover, the approximation error function $A(\lambda)$ is defined by

$$A(\lambda) = \inf_{f \in E} \Omega(h) + R_{L, \lambda}(f) - R_{L, \lambda}. \quad (12)$$

A.1. Error Analysis for $f \in C^{0,\alpha}$

First of all, we introduce some definitions and notations which will be used in the supplementary material. Recall that the $L_p$-distance between $g_1, g_2 \in L_p(\mu)$, $p \in [1, \infty)$, is defined by

$$\|g_1 - g_2\|_{L_p(\mu)} := \left( \int_X |g_1(x) - g_2(x)|^p \, d\mu(x) \right)^{1/p}.$$

For a given histogram transform $H$, let the function set $F_H$ be defined by (3). We write

$$f_{L, \lambda} := \arg \min_{f \in F_H} \|f - \hat{f}\|_{L_2(\mu)}. \quad (13)$$

In other words, $f_{L, \lambda}$ is the function that minimizes the $L_2$-distance over the function set $F_H$ with the bin width $h \in [h_0, \bar{h}_0]$. Then, elementary calculation yields

$$f_{L, \lambda}(x) = \mu_h(\{x \mid A_H(x)\}) = \sum_{j \in I_H} \frac{\int_{A_j} f(x) \, d\mu(x)}{\mu(A_j)} \cdot 1_{A_j}(x)$$

Moreover, we write

$$f_{D, \lambda} = \sum_{j \in I_H} \frac{n_j}{\mu(A_j)} \cdot 1_{A_j}(x) \quad (15)$$

for the empirical version, which can be further presented as

$$f_{D, \lambda} = \sum_{j \in I_H} \frac{D(A_j)}{\mu(A_j)} \cdot 1_{A_j}.$$

Lemma 1 Let $f$ be the underlying probability density function and $P$ is the corresponding distribution of $f$. Moreover, let $L : X \times [0, \infty) \to \mathbb{R}$ be the Negative Log Likelihood loss defined by (1). Then $f$ is exactly the minimizer of $R_{L, \lambda}(\cdot)$ among all density functions. For fixed constants $\xi_f, \bar{\xi}_f \in (0, \infty)$, let $A_0 \subset X$ denote the set

$$A_0 := \{ x \in \mathbb{R}^d : f(x) \in [\xi_f, \bar{\xi}_f] \}. \quad (16)$$

Then for any $x \in A_0$, there holds

$$\frac{\|g - f\|_{L_2(\mu)}^2}{2\xi_f} - \frac{\|g - f\|_{L_2(\mu)}^2}{3\xi_f} \leq R_{L, \lambda}(g) - R_{L, \lambda}(f) \leq \frac{\|g - f\|_{L_2(\mu)}^2}{2\xi_f}.$$

A.1.1. Bounding the Approximation Error Term

The following proposition shows that the $L_2$ distance between $f_{L, \lambda}$ and $f$ behaves polynomial in the regularization parameter $\lambda$ if we choose the bin width $h_0$ appropriately.

Proposition 1 Let the histogram transform $H$ be defined as in (2) with bin width $h$ satisfies Assumption 1. Furthermore, suppose that the density function $f \in C^{0,\alpha}$. Then, for any fixed $\lambda > 0$, there holds

$$\lambda h^{-2d} + R_{L, \lambda}(f_{L, \lambda}) - R_{L, \lambda} \leq c \cdot \lambda^{\frac{\alpha}{1 + \alpha}},$$

where $c$ is some constant depending on $\alpha$, $d$, and $c_0$ as in Assumption 1.

A.1.2. Bounding the Sample Error Term

To derive bounds on the sample error of regularized empirical risk minimizers, let us briefly recall the definition of VC dimension measuring the complexity of the underlying function class.

Definition 2 (VC dimension) Let $B$ be a class of subsets of $X$ and $A \subset X$ be a finite set. The trace of $B$ on $A$ is defined by $\{B \cap A \mid B \subset B\}$. Its cardinality is denoted by $\Delta^B(A)$. We say that $B$ shatters $A$ if $\Delta^B(A) = 2^{\#(A)}$, that is, if for every $A \subset A$, there exists a $B \subset B$ such that $\tilde{A} = B \cap A$. For $k \in \mathbb{N}$, let

$$m^B(k) := \sup_{A \subset X, \#(A) = k} \Delta^B(A). \quad (17)$$
Then, the set $B$ is a Vapnik-Chervonenkis class if there exists $k < \infty$ such that $m_B(k) < 2^k$ and the minimal of such $k$ is called the VC dimension of $B$, and abbreviate as $\text{VC}(B)$.

To prove Lemma 2, we need the following fundamental lemma concerning with the VC dimension of purely random partitions, which follows the idea put forward by (Breiman, 2000) of the construction of purely random forest. To this end, let $p \in \mathbb{N}$ be fixed and $\pi_p$ be a partition of $\mathcal{X}$ with number of splits $p$ and $\pi_{(p)}$ denote the collection of all partitions $\pi_p$.

**Lemma 2** Let $B_p$ be defined by

$$B_p := \left\{ B : B = \bigcup_{j \in J} A_j, J \subset \{0, 1, \ldots, p\}, A_j \in \pi_p \right\}.$$  

(18)

Then the VC dimension of $B_p$ can be upper bounded by $dp + 2$.

To investigate the capacity property of continuous-valued functions, we need to introduce the concept VC-subgraph class. To this end, the subgraph of a function $f : \mathcal{X} \rightarrow \mathbb{R}$ is defined by

$$\text{sg}(f) := \{(x, t) : t < f(x)\}.$$  

A class $\mathcal{F}$ of functions on $\mathcal{X}$ is said to be a VC-subgraph class, if the collection of all subgraphs of functions in $\mathcal{F}$, which is denoted by $\text{sg}(\mathcal{F}) := \{\text{sg}(f) : f \in \mathcal{F}\}$ is a VC class of sets in $\mathcal{X} \times \mathbb{R}$. Then the VC dimension of $\mathcal{F}$ is defined by the VC dimension of the collection of the subgraphs, that is, $\text{VC}(\mathcal{F}) = \text{VC}(\text{sg}(\mathcal{F}))$.

Before we proceed, we also need to recall the definitions of the convex hull and VC-hull class. The symmetric convex hull $\text{Co}(\mathcal{F})$ of a class of functions $\mathcal{F}$ is defined as the set of functions $\sum_{i=1}^m \alpha_i f_i$ with $\sum_{i=1}^m |\alpha_i| \leq 1$ and each $f_i$ contained in $\mathcal{F}$. A set of measurable functions is called a VC-hull class, if it is in the pointwise sequential closure of the symmetric convex hull of a VC-class of functions.

We denote the function set $\mathcal{F}$ as

$$\mathcal{F} := \bigcup_{H \sim \mathcal{P}_H} \mathcal{F}_H,$$

(19)

which contains all the functions of $\mathcal{F}_H$ induced by histogram transforms $H$ with bin width $L_0$.

The following lemma presents the upper bound for the VC dimension of the function set $\mathcal{F}$.

**Lemma 3** Let $\mathcal{F}$ be the function set defined as in (19). Then $\mathcal{F}$ is a VC-subgraph class with

$$\text{VC}(\mathcal{F}) \leq (d + 1)2^{d+1}\left(\left\lfloor 2R\sqrt{d}/L_0 \right\rfloor + 1\right)^d.$$  

To further bound the capacity of the function sets, we need to introduce the following fundamental descriptions which enables an approximation of an infinite set by finite subsets.

**Definition 3 (Covering Numbers)** Let $(\mathcal{X}, d)$ be a metric space, $A \subseteq \mathcal{X}$ and $\varepsilon > 0$. We call $A' \subseteq A$ an $\varepsilon$-net of $A$ if for all $x \in A$ there exists an $x' \in A'$ such that $d(x, x') \leq \varepsilon$. Moreover, the $\varepsilon$-covering number of $A$ is defined as

$$\mathcal{N}(A, d, \varepsilon) = \inf \left\{ n \geq 1 : \exists x_1, \ldots, x_n \in \mathcal{X}, \right.$$  

$$\text{such that } A \subset \bigcup_{i=1}^n B_d(x_i, \varepsilon) \right\},$$

where $B_d(x, \varepsilon)$ denotes the closed ball in $\mathcal{X}$ centered at $x$ with radius $\varepsilon$.

The following lemma follows directly from Theorem 2.6.9 in (Van der Vaart & Wellner, 1996). For the sake of completeness, we present the proof in Section B.1.2.

**Lemma 4** Let $Q$ be a probability measure on $\mathcal{X}$ and

$$\mathcal{F} := \{ f : \mathcal{X} \rightarrow \mathbb{R} : f \in [-M, M] \}.$$  

Assume that for some fixed $\varepsilon > 0$ and $v > 0$, the covering number of $\mathcal{F}$ satisfies

$$\mathcal{N}(\mathcal{F}, L_2(Q), M\varepsilon) \leq c (1/\varepsilon)^v.$$  

(20)

Then there exists a universal constant $c'$ such that

$$\log \mathcal{N}(\text{Co}(\mathcal{F}), L_2(Q), M\varepsilon) \leq c'v^{2/(v+2)}\varepsilon^{-2v/(v+2)}.$$  

The next theorem shows that covering numbers of $\mathcal{F}$ grow at a polynomial rate.

**Theorem 4** Let $\mathcal{F}$ be a function set defined as in (19). Then there exists a universal constant $c < \infty$ such that for any $\varepsilon \in (0, 1)$ and any probability measure $Q$, we have

$$\mathcal{N}(\mathcal{F}, L_2(Q), M\varepsilon) \leq c_0 \left(\frac{cd/L_0}{d}d\right)^d \cdot (16c)^{cd/L_0} \varepsilon^{2L_0/(cd)}d^{-2},$$

where the constant $c_0 := 2^{1+4/d} \cdot d^{1/2+1/d}$.

The following theorem gives an upper bound on the covering number of the VC-hull class $\text{Co}(\mathcal{F})$.

**Theorem 5** Let $\mathcal{F}$ be the function set defined as in (19). Then there exists a constant $c_1$ such that for any $\varepsilon \in (0, 1)$ and any probability measure $Q$, there holds

$$\log \mathcal{N}(\text{Co}(\mathcal{F}), L_2(Q), M\varepsilon) \leq c_1 \varepsilon^{2L_0/(cd)}d^{-2}.$$  

(21)

Next, let us recall the definition of entropy numbers.
Moreover, if \( C \) we turn to the function space \( f \) a point in introducing some notations. As a result, we fail to prove the exact benefits expansion involved techniques for error estimation may not more, let \( f \in (2) \) be the GBHT defined by Definition 4 (Entropy Numbers). Let the histogram transform \( E \) identity map that assigns to every \( f \) \( \Omega(\lambda) \) be as in Section 3.3. Then for any \( P^n \otimes P_H \) not less than \( 1 - 3e^{-\tau} \), we have

\[
\Omega(h) + \mathcal{R}_{L,D}(f_D,\lambda) - \mathcal{R}_{L,P}^* \leq 12\lambda + 3456M^2\tau/n + 3c_0\lambda^{-\frac{1}{1+2\gamma}}n^{-\frac{2}{1+2\gamma}},
\]

where \( c_0^* \) is a constant.

A.2. Error Analysis for \( f \in C^{1,\alpha} \)

A drawback to the analysis in \( C^{0,\alpha} \) is that the usual Taylor expansion involved techniques for error estimation may not apply directly. As a result, we fail to prove the exact benefits of the boosting procedure. Therefore, in this subsection, we turn to the function space \( C^{1,\alpha} \) consisting of smoother functions. To be specific, we study the convergence rates of \( f_D,\lambda \) to the density function \( f \in C^{1,\alpha} \). To this end, there is a point in introducing some notations.

For fixed \( b_0, b_0, h_0 > 0 \), let \( \{H_t\}_{T=1}^T \) be histogram transforms with bin width \( h_t \in [b_0, b_0] \), \( t = 1, \ldots, T \). Moreover, let \( \{f_P, H_t\}_{T=1}^T \) and \( \{f_P, H_t\}_{T=1}^T \) be defined as in (13) and (15), respectively. For \( x \in \mathcal{X} \), we define

\[
f_{P,E}(x) := \frac{1}{T} \sum_{t=1}^T f_{P,H}(x)
\]

and

\[
f_{P,D,E}(x) := \frac{1}{T} \sum_{t=1}^T f_{D,H}(x).
\]

Then we make the error decomposition

\[
\mathbb{E}_{\nu_n} ||f_{D,E} - f||_{L^2(\mu)}^2 = \mathbb{E}_{\nu_n} ||f_{D,E} - f_{P,E}||_{L^2(\mu)}^2 + \mathbb{E}_{\nu_n} ||f_{P,E} - f||_{L^2(\mu)}^2.
\]

A.2.2 Upper Bound for Convergence Rate of GBHT

The following Lemma presents the explicit representation of \( A_H(x) \) which will be used later in the proofs of Proposition 2.

**Lemma 5** Let the histogram transform \( H \) be defined as in (2) and \( A^*_H \) be as in Section 3.3. Then for any \( x \in \mathbb{R}^d \), the set \( A^*_H(x) \) can be represented as

\[
A_H(x) = \{x + (R \cdot S)^{-1} z : z \in [-b', 1 - b'] \},
\]

where \( b' \sim \text{Unif}(0, 1)^d \).
The next proposition presents the upper bound of the $L_2$ distance between GBHT $f_{P, R}$ (22) and the density function $f$ in the Hölder space $C^{1, \alpha}$.

**Proposition 2** Let the histogram transform $H$ be defined as in (2) with bin width $h$ satisfying Assumption 1 and $T$ be the number of iterations. Furthermore, let $P_X$ be the uniform distribution and $L_{\pi_0}(x, y, t)$ be the restricted negative log-likelihood loss defined as in (9). Moreover, let the density function satisfy $f \in C^{1, \alpha}$. For fixed constants $\xi_f, \tau_f \in (0, \infty)$, let $A_f^j$ be as in (16). Then for any $x \in A_f^j$, there holds

$$\mathcal{R}_{L_{\pi_0}, P}(f_{P, R}) - \mathcal{R}_{L_{\pi_0}, P} \leq \frac{c_f^2 \mu(B_R)}{2L_f} \left( \frac{\kappa^2(1+\alpha)}{h} + \frac{d}{T} \cdot h_0 \right)$$

(27)

in expectation with respect to $P_H$. 

**A.2.2. Lower Bound of $L_2$-Convergence Rate of HT**

**Theorem 7** Let the histogram transform $H_n$ be defined as in (2) with bandwidth $h_n$ satisfying Assumption 1. Furthermore, let the density function $f \in C^{1, \alpha}$. For fixed constants $\xi_f, \tau_f, \xi_f^\prime \in (0, \infty)$, let $A_f^j$ denote the set

$$A_f^j := \left\{ x \in \mathbb{R}^d : \| \nabla f \|_{\infty} \geq \xi_f^\prime \text{ and } f(x) \in [\xi_f, \tau_f] \right\}.$$  

(28)

If $\mu(B_R^\prime \cap A_f^j) > 0$, then for all $n > N_0$ with

$$N_0 := \min \left\{ n \in \mathbb{N} : \mathcal{T}_0, n \leq \min \left\{ \left( \frac{\sqrt{dc_f^2} c_0 n}{4 \sqrt{3c_L}} \right)^{\frac{1}{\alpha}}, \left( \frac{d \sqrt{\sigma}}{2} \right)^{\frac{1}{\alpha}} c_f \frac{1}{2d \sqrt{\sigma c_L}} \right\} \right\},$$

(29)

by choosing

$$\mathcal{T}_0, n := n^{-\frac{1}{2+\alpha}},$$

there holds

$$\| f_{D, H} - f \|_{L_2(\nu_n)}^2 \gtrsim n^{-\frac{2}{2+\alpha}}$$

(30)

in the sense of $L_2(\nu_n)$-norm.

In order to prove Theorem 7, we prove the following two propositions presenting the lower bound of approximation error and sample error of HT respectively.

**Proposition 3** Let the histogram transform $H$ be defined as in (2) with bin width $h$ satisfying Assumption 1 and $\mathcal{T}_0 \leq 1$. Moreover, let the density function $f \in C^{1, \alpha}(B_R)$. For a fixed constant $\xi_f \in (0, \infty)$, let $A_f^j$ be the set (28). Let $N_1$ be defined as

$$N_1 := \min \left\{ n \in \mathbb{N} : \mathcal{T}_0, n \leq \left( \frac{\sqrt{dc_f^2} c_0 n}{4 \sqrt{3c_L}} \right)^{\frac{1}{\alpha}} \right\}.$$  

(31)

Then for all $n > N_1$, there holds

$$\| f_{P, H} - f \|_{L_2(\nu_n)}^2 \gtrsim \frac{d}{16} \mu(A_f^j \cap B_{R, \sqrt{d} h_0}) \xi_f \tau_f^2 \cdot h_0.$$  

(32)

in expectation with respect to $P_H$. 

**Proposition 4** Let the histogram transform $H_n$ be defined as in (2) with bandwidth $h_n$ satisfying Assumption 1. Moreover, let the density function $f \in C^{1, \alpha}$ and $A_f^j$ be the set (28). Then for all $x \in B_{R, \sqrt{d} h_0} \cap A_f^j$ and all $n \geq N'$ with

$$N' := \min \left\{ n \in \mathbb{N} : \mathcal{T}_0, n \leq \min \left\{ \left( \frac{d \sqrt{\sigma}}{2} \right)^{\frac{1}{\alpha}} c_f \frac{1}{2d \sqrt{\sigma c_L}} \right\} \right\},$$

there holds

$$\| f_{D, H} - f_{P, H} \|_{L_2(\mu)}^2 \gtrsim \mu(A_f^j \cap B_{R, \sqrt{d} h_0}) \xi_f \tau_f^2 \cdot h_0, n^{-1}$$

(33)

in expectation with respect to $P^n$.

**A.2.3. Upper Bound of $L_2$-Convergence Rate of HT**

**Proposition 5** Let the histogram transform $H_n$ be defined as in (2) with bandwidth $h_n$ satisfying Assumption 1. Furthermore, let the density function $f \in C^{1, \alpha}$ and for fixed constants $\xi_f, \tau_f, \xi_f^\prime \in (0, \infty)$, let $A_f^j$ be the set (28). Then for all $n > N_0$ with $N_0$ as in (29), there holds

$$\| f_{D, H} - f \|_{L_3(\mu)}^3 \leq \mu(B_{R, \sqrt{d} h_0} \cap A_f^j) \cdot \left( \frac{dc_f^2}{4} \cdot h_0 \right)^{3+\alpha}$$

$$+ c_\alpha \cdot \mathcal{T}_0, n^{-1} \cdot h_0^{2d}$$

$$+ 3c_f^2 \cdot n^{-1} \cdot h_0^{d+1+\alpha},$$

where $c_\alpha$ is some constant depending on $\alpha$.

**B. Proofs**

It is well-known that entropy numbers are closely related to the covering numbers. To be specific, entropy and covering numbers are in some sense inverse to each other. More precisely, for all constants $a > 0$ and $q > 0$, the implication

$$e_i(T, d) \leq a_i^{-1/q}, \quad \forall i \geq 1$$

$$\implies \ln \mathcal{N}(T, d, \varepsilon) \leq \ln(4)(a/\varepsilon)^q, \quad \forall \varepsilon > 0$$

(34)

(35)
holds by Lemma 6.2 in (Steinwart & Christmann, 2008). Additionally, Exercise 6.8 in (Steinwart & Christmann, 2008) yields the opposite implication, namely
\[
\ln N(T, d, \varepsilon) < (a/\varepsilon)^q, \quad \forall \varepsilon > 0 \implies e_i(T, d) \leq 3^{1/q}a^{-1/q}, \quad \forall i \geq 2 \frac{g(x) - f(x)}{f(x)} - \frac{1}{2} E_p \left( \frac{g(x) - f(x)}{f(x)} \right)^2
\]
Using (37), we get
\[
E_p \left[ 1 + \frac{g(x) - f(x)}{f(x)} \right] \leq \frac{1}{3} E_p \left( \frac{g(x) - f(x)}{f(x)} \right)^3.
\]
Combining (39) with (38), we obtain
\[
E_p \log \left( 1 + \frac{g(x) - f(x)}{f(x)} \right) \leq \frac{1}{2} E_p \left( \frac{g(x) - f(x)}{f(x)} \right)^2 - \frac{1}{3} E_p \left( \frac{g(x) - f(x)}{f(x)} \right)^3.
\]
Consequently, for any \( x \) satisfying \( f(x) \in [\varepsilon_f, \tau_f] \), there holds
\[
\mathcal{R}_{L,P}(g) - \mathcal{R}_{L,P}(f) \geq \frac{\|g - f\|_{L^2(\mu)}^2 - \|g - f\|_{L^2(\mu)}^2}{3\varepsilon_f^2},
\]
which completes the proof.

**Proof 1 (Proof of Lemma 1) For any density function \( g \), there holds**
\[
\mathcal{R}_{L,P}(g) - \mathcal{R}_{L,P}(f) = -E_p \log g(X) + E_p \log f(X)
\]
\[
= -E_p \log \left( \frac{g(x)}{f(x)} \right)
\]
\[
= -E_p \log \left( 1 + \frac{g(x) - f(x)}{f(x)} \right).
\]
Using \( x - x^2/2 \leq \log(1 + x) \leq x, x > -1 \), we get
\[
E_p \frac{g(x) - f(x)}{f(x)} \leq \mathcal{R}_{L,P}(g) - \mathcal{R}_{L,P}(f)
\]
\[
\leq E_p \frac{g(x) - f(x)}{f(x)} + E_p \left( \frac{g(x) - f(x)}{f(x)} \right)^2 - 2f(x)^2.
\]
Since \( g \) is a density function, we have
\[
E_p \frac{g(x) - f(x)}{f(x)} = \int_X \frac{g(x) - f(x)}{f(x)} f(x) dx
\]
\[
= \int_X g(x) dx - \int_X f(x) dx = 1 - 1 = 0.
\]
On the one hand, (38) together with the first inequality in (37) yields
\[
\mathcal{R}_{L,P}(g) - \mathcal{R}_{L,P}(f) \geq 0.
\]
Moreover, the equation holds if and only if \( g = f \). On the other hand, combining the second inequality (37) and (38), we obtain
\[
\mathcal{R}_{L,P}(g) - \mathcal{R}_{L,P}(f)
\]
\[
\leq E_p \frac{(g(x) - f(x))^2}{2f(x)^2} = \int_X \frac{(g(x) - f(x))^2}{2f(x)} d\mu(x).
\]
Thus, for all \( x \) satisfying \( f(x) \geq \varepsilon_f \), we have
\[
\mathcal{R}_{L,P}(g) - \mathcal{R}_{L,P}(f) \leq \frac{\|f - g\|_{L^2(\mu)}^2}{2\varepsilon_f}.
\]
We proceed by induction. Firstly, we concentrate on partitioning. Concretely, owing to the fact that \( d \) is the dimension of the feature space, the smallest number of sample points that cannot be divided by \( p = 1 \) split is \( d + 2 \). Inductively, the above analysis can be extended to the general case of \( d \)-dimensional space, in which we might take the following case into consideration: There is a hyperplane consisting of \( d \) points all from one class, say class \( A \), and two points \( p_1^B, p_2^B \) from the opposite class \( B \) located on the opposite sides of this hyperplane, respectively. We denote this hyperplane by \( H_{1}^{A} \). In this case, points from two classes cannot be separated by one split (since the positions are \( p_1^B, H_{1}^{A}, p_2^B \)), so that we have \( \text{VC}(B_1) \leq d + 2 \).

Next, when the partition is with the number of splits \( p = 2 \), we analyze in the similar way only by extending the above case a little bit. Now, we pick either of the two single sample points located on opposite side of the \( H_{1}^{A} \), and add \( d - 1 \) more points from class \( B \) to it. Then, they together can form a hyperplane \( H_{2}^{B} \) parallel to \( H_{1}^{A} \). After that, we place one more sample point from class \( A \) to the side of this newly constructed hyperplane \( H_{2}^{B} \). In this case, the number of these two sample points and two hyperplanes are \( p_1^B, H_{1}^{A}, H_{2}^{B}, p_2^B \). Apparently, \( p = 2 \) splits cannot separate these \( 2d + 2 \) points. As a result, we have \( \text{VC}(B_2) \leq 2d + 2 \).

Inductively, the above analysis can be extended to the general case of \( d \)-dimensional space, in which we need to add points continuously to form \( p \) mutually parallel hyperplanes where any two adjacent hyperplanes should be constructed from different classes. Without loss of generality, we consider the case for \( p = 2k + 1, k \in \mathbb{N} \), where two points (denoted as \( p_1^B, p_2^B \)) from class \( B \) and \( 2k + 1 \) alternately appearing hyperplanes form the space locations: \( p_1^B, H_{1}^{A}, H_{2}^{B}, H_{1}^{A}, H_{2}^{B}, \ldots, H_{2k+1}^{A}, p_2^B \). Accordingly, the smallest number of points that cannot be divided by \( p \) splits is \( dp + 2 \), leading to \( \text{VC}(B_p) \leq dp + 2 \). This completes the proof.

**Proof 4 (Proof of Lemma 3)** Recall that for a histogram transform \( H \), the set \( \pi_H = (A_j)_{j \in \mathbb{I}_H} \) is a partition of \( B_R \) with the index set \( \mathbb{I}_H \) induced by \( H \). The choice \( k := \lfloor 2R\sqrt{d/h_0} \rfloor + 1 \) leads to the partition of \( B_R \) of the form \( \pi_k := \{A_{i_1, \ldots, i_d}\}_{j=1, \ldots, k} \) with

\[
A_{i_1, \ldots, i_d} := \prod_{j=1}^{d} A_j
\]

\[
:= \prod_{j=1}^{d} \left( -R + \frac{2R(i_j - 1)}{k}, -R + \frac{2Ri_j}{k} \right).
\]

(41)

Obviously, we have \( |A_{i_j}| \leq \frac{h_0}{\sqrt{d}} \). Let \( D \) be a data set of the form

\[
D := \{(x_i, t_i) : x_i \in B_R, t_i \in [-M, M], i = 1, \ldots, m \}
\]

with

\[
m := \#(D) = 2^{d+1}(d + 1)(\lfloor 2R\sqrt{d/h_0} \rfloor + 1)^d.
\]

Then there exists at least one cell \( A \) with

\[
\#(D \cap (A \times [-M, M])) \geq 2^{d+1}(d + 1).
\]

Moreover, for any \( x, x' \in A \), the construction of the partition (41) implies \( \|x - x'\| \leq h_0 \). Consequently, for any arbitrary histogram transform \( H \) and \( A_j \in \pi_H \), at most one vertex of \( A_j \) lies in \( A \), since the bin width of \( A_j \) is larger than \( h_0 \). Therefore,

\[
\Pi_{H|A} := \left\{ \bigcup_{j \in I} ((A_{j} \cap A) \times [-M, c_j]), I \subset \mathbb{I}_H \right\} \cup \left\{ \bigcup_{j \in I} ((A_{j} \cap A) \times (c_j, M]), I \subset \mathbb{I}_H \right\}
\]

forms a partition of \( A \times [-M, M] \) with \( \#(\Pi_{H|A}) \leq 2^{d+1} \).

It is easy seen that this partition can be generated by \( 2^{d+1} - 1 \) splitting hyperplanes on the space \( A \times [-M, M] \). In this way, Lemma 2 implies that \( \Pi_{H|A} \) can only shatter a dataset with at most \( (d + 1)(2^{d+1} - 1) + 1 \) elements. Thus (42) indicates that \( \Pi_{H|A} \) fails to shatter \( D \cap (A \times [-M, M]) \).

Therefore, the subgraphs of \( F \)

\[
\{ \{(x, t) : t < f(x)\}, f \in F \}
\]

cannot shatter the data set \( D \) as well. By Definition 2, we immediately get

\[
\text{VC}(F) \leq 2^{d+1}(d + 1)(\lfloor 2R\sqrt{d/h_0} \rfloor + 1)^d
\]

and the assertion is thus proved.

**Proof 5 (Proof of Lemma 4)** Let \( F_\varepsilon \) be an \( \varepsilon \)-net over \( F \). Then, for any \( f \in \text{Co}(F) \), there exists an \( f_\varepsilon \in \text{Co}(F_\varepsilon) \)
such that $\|f - f_1\|_{L_2(Q)} \leq \varepsilon$. Therefore, we can assume without loss of generality that $F$ is finite.

Obviously, (20) holds for $1 \leq \varepsilon \leq c_1^{1/v}$. Let $v' := 1/2 + 1/v$ and $M' := c_1^{1/v}M$. Then (20) implies that for any $n \in \mathbb{N}$, there exists $f_1, \ldots, f_n \in F$ such that for any $f \in F$, there exists an $f_1$ such that

$$\|f - f_1\|_{L_2(Q)} \leq M' n^{-1/v}.$$  

Therefore, for each $n \in \mathbb{N}$, we can find sets $F_1 \subset F_2 \subset \cdots \subset F$ such that the set $F_n$ is a $M' n^{-1/v}$-net over $F$ and $\#(F_n) \leq n$.

In the following, we show by induction that for $q \geq 3 + v$ and $n, k \geq 1$, there holds

$$\log N(\text{Co}(F_{nk}), L_2(Q), c_k M' n^{-v'}) \leq c_k' n,$$  

where $c_k$ and $c_k'$ are constants depending only on $c$ and $v$ such that $\sup_k \max\{c_k, c_k'\} < \infty$. The proof of (43) will be conducted by a nested induction argument.

Let us first consider the case $k = 1$. For a fixed $n_0$, let $n \leq n_0$. Then for $c_1$ satisfying $c_1 M' n_0^{-v'} \geq M$, there holds

$$\log N(\text{Co}(F_{nk}), L_2(Q), c_1 M' n^{-v'}) = 0,$$  

which immediately implies (43). For a general $n \in \mathbb{N}$, let $m := n/\ell$ for large enough $\ell$ to be chosen later. Then for any $f \in F_n \setminus F_m$, there exists an $f^{(m)} \in F_m$ such that

$$\|f - f^{(m)}\|_{L_2(Q)} \leq M' m^{-1/v}.$$  

Let $\pi_m : F_n \setminus F_m \rightarrow F_m$ be the projection operator. Then for any $f \in F_n \setminus F_m$, there holds

$$\|f - \pi_m f\|_{L_2(Q)} \leq M' m^{-1/v}.$$  

Therefore, for $\lambda_i, \mu_j \geq 0$ and $\sum_{i=1}^n \lambda_i = \sum_{j=1}^m \mu_j = 1$, we have

$$\sum_{i=1}^n \lambda_i f_i^{(n)} = \sum_{j=1}^m \mu_j f_j^{(m)} + \sum_{k=m+1}^n \lambda_k (f_k^{(n)} - \pi_m f_k^{(n)}).$$  

Let $G_n$ be the set

$$G_n := \{0\} \cup \{f - \pi_m f : f \in F_n \setminus F_m\}.$$  

Then we have $\#(G_n) \leq n$ and for any $g \in G_n$, there holds

$$\|g\|_{L_2(Q)} \leq M' m^{-1/v}.$$  

Moreover, we have

$$\text{Co}(F_n) \subset \text{Co}(F_m) + \text{Co}(G_n).$$  

(44)

Applying Lemma 2.6.11 in (Van der Vaart & Wellner, 1996) with $w := \frac{1}{2} c_1 M' m^{-v'}$ to $G_n$, we can find a $\frac{1}{2} c_1 M' n^{-v'}$-net over $\text{Co}(G_n)$ consisting of at most

$$(e + e n^{2v'} / 2 \ell)^{2\ell^{2v'}} c_1^{-2n}$$  

(45)

elements.

Suppose that (43) holds for $k = 1$ and $n = m$. In other words, there exists a $c_1 M' m^{-v'}$-net over $\text{Co}(F_m)$ consisting of at most $e^m$ elements, which partitions $\text{Co}(F_m)$ into $m$-dimensional cells of diameter at most $2 c_1 M' m^{-v'}$. Each of these cells can be isometrically identified with a subset of a ball of radius $c_1 M' m^{-v'}$ in $\mathbb{R}^m$ and can be therefore further partitioned into

$$\left(\frac{3 c_1 M' m^{-v'}}{\frac{1}{2} c_1 M' n^{-v'}}\right)^m = (6e')^{n/\ell}$$  

(46)

cells of diameter $\frac{1}{2} c_1 M' n^{-v'}$. As a result, we get a $\frac{1}{2} c_1 M' n^{-v'}$-net of $\text{Co}(F_m)$ containing at most

$$e^m \cdot (6e')^{n/\ell}$$  

(47)

elements.

Now, (44) together with (45) and (46) yields that there exists a $c_1 M' n^{-v'}$-net of $\text{Co}(F_n)$ whose cardinality can be bounded by

$$e^{n/\ell} (6e')^{n/\ell} \left(e + \frac{ee_1}{\ell^{2v'}} \right)^{2\ell^{2v'} c_1^{-2n}} \leq e^n,$$  

where $G_n$.
for suitable choices of $c_1$ and $\ell$ depending only on $v$. This concludes the proof of (43) for $k = 1$ and every $n \in \mathbb{N}$.

Let us consider a general $k \in \mathbb{N}$. Similarly as above, there holds
\[
\text{Co}(\mathcal{F}_{n_k}) \subset \text{Co}(\mathcal{F}_{n(k-1)^v}) + \text{Co}(\mathcal{G}_{n,k}), \tag{47}
\]
where the set $\mathcal{G}_{n,k}$ contains at most $nk^q$ elements with norm smaller than $M'(n(k-1)^{1/v})^{-1/v}$. Applying Lemma 2.6.11 in (Van der Vaart & Wellner, 1996), we can find an $M'_k(n^{-v'}-\text{net over Co}(\mathcal{G}_{n,k})$ consisting of most
\[
(e + e(k^{2q/v-4+q})^{2q/v+1}k^{4-2q/v}n
\]
elem. Moreover, by the induction hypothesis, we have a $c_{k-1}M'_k(n^{-v'})\text{-net over Co}(\mathcal{F}_{(n(k-1)^v})$ consisting of at most $e^{c_{k-1}n}$ elements. Using (47), (48), and (49), we obtain a $c_kM'_k(n^{-v'})\text{-net over Co}(\mathcal{F}_{n(k-1)^v})$ consisting of at most $e^{c_kn}$ elements, where
\[
c_k = c_k + 1/k^2, \\
c'_k = c_k + 2^{2q/v+1}1 + \log(1 + k^{2q/v-4+q})/k^{2q/v-4}.
\]
Form the elementary analysis we know that if $2q/v - 5 = 2$, then there exist constants $c'_1, c'_2,$ and $c'_3$ such that
\[
\lim_{k \to \infty} c_k = c^{-1/v}n_0^{(v+2)/2v} + \sum_{i=2}^{\infty} 1/i^2 \leq c'_1e^{-1/v} + c'_2, \\
\lim_{k \to \infty} c'_k = 1 + \sum_{i=1}^{\infty} 2(2/i)^{2q/v} \leq c'_3.
\]
Thus (43) is proved. Taking $\varepsilon := c_kM'_k(n^{-v'})/M$ in (43), we get
\[
\log N(\text{Co}(\mathcal{F}_{n_k}), L_2(Q), M\varepsilon) \leq c'_ke^{1/v'}(M^1/v')^{-1/v'}. \\
\text{This together with}
\[
(M^1/v') = (c^{1/v}M)^{1/v'} = e^{2/(v+2)}M^{1/v'}
\]
yields
\[
\log N(\text{Co}(\mathcal{F}), L_2(Q), M\varepsilon) \leq c'e^{2/(v+2)}e^{-2/v'(v+2)},
\]
where the constant $c'$ depends on the constants $c'_1, c'_2$ and $c'_3$. This finishes the proof.

**Proof 6 (Proof of Theorem 4)** We find the upper bound of $\text{VC}(\mathcal{F})$ satisfies
\[
2^{d+1}(d + 1)(2R\sqrt{d}/h_0 + 2)^d \leq d \cdot 2^{d+2}(4R\sqrt{d}/h_0)^d = (c_dR/h_0)^d,
\]
where $c_d := 2^{1+4/d} \cdot d^{1+2+1/d}$. Then Theorem 2.6.7 in (Van der Vaart & Wellner, 1996) yields the assertion.

**Proof 7 (Proof of Theorem 5)** The assertion follows directly from Lemma 4 with
\[
c := c_0(c_d/h_0)^d \cdot (16e)(c_d/h_0)^d, \quad v := 2((c_d/h_0)^d - 1).
\]
Let $\delta := (h_0/c_d)^d$, then we have
\[
c^{2/(v+2)} = (c_0\delta^{-1}(16e)^{1/\delta}) = 16e(c_0\delta^{-1})^{\delta} = 16e(c_0\delta^{-1})^{\delta}.
\]
Note that the function $f$ defined by $f(\delta) := (c_0\delta^{-1})^{\delta}$ is continuous and
\[
\lim_{\delta \to 0} f(\delta) = 1.
\]
Then there exists a constant $M_d > 0$ such that $f(\delta) \leq M_d$ for all $0 < \delta \leq (1/c_d)^d$ if $h_0 \leq 1$. Consequently, we have
\[
\log N(\text{Co}(\mathcal{F}), L_2(Q), M\varepsilon) \leq 16ec'M_d e^{2(h_0/c_d)^d - 2}.
\]
With $c_1 := 16ec'M_d$ we obtain the assertion.

**Definition 5** Let $f$ be density function and $P$ be the corresponding probability distribution on $\mathcal{X}$. For a loss function $L: \mathcal{X} \times [0, \infty] \to \mathbb{R}$ and denote $L \circ g := L(x, g(x))$, Then $L$ satisfies the supreme bound and variance bound if there exist constants $B > 0, \theta \in [0, 1]$ and $V \geq B^2 - \theta$ such that for any function $g$, there holds
\[
\|L \circ g - L \circ f\|_{\infty} \leq B,
\]
\[
E_P(L \circ g - L \circ f)^2 \leq V \cdot (E_P(L \circ g - L \circ f))^\theta.
\]

**Lemma 6** Let $L$ be the negative log-likelihood loss defined in (1). Moreover, let $f$ be the underlying density function of the probability distribution $P$ on $B_R$ satisfying $c_f \leq f(x) \leq \tau_f$ for all $x \in B_R$. Then for any $g$ with $c_f \leq g(x) \leq \tau_f$, $L$ satisfies the supreme bound and variance bound in Definition 5 with $B = 2\max\{|\log c_f|, |\log \tau_f|\}$ and $V = 2\max\{|\log c_f|, |\log \tau_f|\}$, $\theta = 1$.

**Proof of Lemma 6** First any $x \in B_R$, there holds
\[
\|L \circ g - L \circ f\|_{\infty} \leq \max_{x \in B_R} \log |f(x)| + \max_{x \in B_R} \log |g(x)| \leq 2\max\{|\log c_f|, |\log \tau_f|\} =: B.
\]
Using Taylor’s expansion, we get
\[
\begin{align*}
\mathbb{E}_p(L \circ g - L \circ f)^2 &= \mathbb{E}_p(- \log g(x) + \log f(x))^2 \\
&= \mathbb{E}_p\left(- \log \left(1 + \frac{g(x) - f(x)}{f(x)}\right)\right)^2 \\
&\leq \mathbb{E}_p\left(\frac{g(x) - f(x)}{f(x)} - \frac{(g(x) - f(x))^2}{2f(x)^2}\right)^2 \\
&= \mathbb{E}_p\left(\frac{(g(x) - f(x))^2}{f(x)} - \frac{(g(x) - f(x))^3}{f(x)}\right) + o\left(\frac{(g(x) - f(x))^3}{f(x)}\right),
\end{align*}
\]
and
\[
\begin{align*}
\mathbb{E}_p(L \circ g - L \circ f) &= \mathbb{E}_p\left(- \log \left(1 + \frac{g(x) - f(x)}{f(x)}\right)\right) \\
&= \mathbb{E}_p\left(- \frac{g(x) - f(x)}{f(x)} + \frac{1}{2} g(x) - f(x)\right)^2 \\
&\quad - \frac{1}{3}\left(\frac{g(x) - f(x)}{f(x)}\right)^3 + o\left(\left(\frac{g(x) - f(x)}{f(x)}\right)^3\right) \\
&= \mathbb{E}_p\left(\frac{1}{2} \frac{(g(x) - f(x))^2}{f(x)} - \frac{1}{3}\left(\frac{g(x) - f(x)}{f(x)}\right)^3\right) + o\left(\left(\frac{g(x) - f(x)}{f(x)}\right)^3\right).
\end{align*}
\]
where the last inequality follows from
\[
\begin{align*}
\mathbb{P}\left(\frac{(g(x) - f(x))}{f(x)}\right) &= \int_{B_R} \frac{g(x) - f(x)}{f(x)} f(x) \, dx \\
&= \int_{B_R} g(x) - f(x) \, dx \\
&= \int_{B_R} g(x) \, dx - \int_{B_R} f(x) \, dx = 0.
\end{align*}
\]
Consequently we have
\[
\mathbb{E}_p(L \circ g - L \circ f)^2 \leq 2\mathbb{E}_p(L \circ g - L \circ f).
\]
Choosing \( V := \max\{2, B\} = 2\max\{1, |\log \xi_f|, |\log \tau_f|\} \), we obtain the assertion.

**Proof 9 (Proof of Theorem 6)** Denote
\[
r^* := \Omega(h) + \mathcal{R}_{L,p}(f) - \mathcal{R}_{L^*,p}^*,
\]
and for \( r > r^* \), we write
\[
\mathcal{F}_r := \{ f \in E : \Omega(h) + \mathcal{R}_{L,p}(f) - \mathcal{R}_{L^*,p}^* \leq r \},
\]
\[
\mathcal{H}_r := \{ L \circ f - L \circ f^*_{L,p} : f \in \mathcal{F}_r \}.
\]
Note that for \( f \in \mathcal{F}_r \), we have \( f = \sum_{t=1}^T w_t f_t \), where \( f_t \in \mathcal{F} \) and \( \sum_{t=1}^T w_t = 1 \). Consequently, we have \( \mathcal{F}_r \subset \text{co}(\mathcal{F}) \).

Since \( L \) is Lipschitz continuous with \( |L|_1 \leq \xi_f^{-1} \), we find
\[
\mathbb{E}_{D \sim P^n} e_m(\mathcal{H}_r, L_2(D)) \leq \xi_f^{-1} \mathbb{E}_{D \sim P^n} e_m(\mathcal{F}_r, L_2(D)) \leq 2\xi_f^{-1} \mathbb{E}_{D \sim P^n} e_m(\text{co}(\mathcal{F}), L_2(D)).
\]
Let \( \delta := (\log c_d/d)^d \), \( \delta' := 1 - \delta \), and \( a := c_1^{1/(2\delta')} M \). Then (21) together with (36) implies that
\[
e_m(\text{co}(\mathcal{F}), L_2(D)) \leq (3c_1)^{1/(2\delta')} M^{-1/2\delta'},
\]
Taking expectation with respect to \( P^n \), we get
\[
\mathbb{E}_{D \sim P^n} e_m(\text{co}(\mathcal{F}), L_2(D)) \leq c_2 a^{-1/2\delta'},
\]
which \( c_2 := (3c_1)^{1/(2\delta')} M \). Moreover, we easily find
\[
\lambda h^{-2d} = \Omega(h) \leq \Omega(f) + \mathcal{R}_{L,p}(f) - \mathcal{R}_{L^*,p}^* \leq r,
\]
which yields
\[
\lambda h^{-2d} \leq (r/\lambda)^{1/(2d)}.
\]
Therefore, if \( \lambda \leq 1 \), then we have \( r \geq \lambda \geq 1 \) and (50) can be further estimated by
\[
\mathbb{E}_{D \sim P^n} e_m(\mathcal{H}_r, L_2(D)) \leq c_2 (r/\lambda)^{1/(4\delta')} M^{-1/2\delta'},
\]
which leads to
\[
\mathbb{E}_{D \sim P^n} e_m(\mathcal{H}_r, L_2(D)) \leq c_2 a^{-1} (r/\lambda)^{1/(4\delta')} M^{-1/2\delta'}.
\]
For the negative log-likelihood loss \( L \), Lemma 6 implies the supreme bound
\[
L(x, t) \leq 2 \max\{|\log \xi_f|, |\log \tau_f|\}, \quad \forall x \in B_R, \ t \in [\xi_f, \tau_f],
\]
and the variance bound
\[
\mathbb{E}(L \circ g - L \circ f)^2 \leq \mathbb{E}(V(E(L \circ g - L \circ f^*_{L,p}))^0
\]
holds for \( V = 2 \max\{1, |\log \xi_f|, |\log \tau_f|\} \) and \( \vartheta = 1 \).
Therefore, for \( h \in \mathcal{H}_r \), we have
\[
\|h\|_\infty \leq 4 \max\{|\log \xi_f|, |\log \tau_f|\},
\]
\[
\mathbb{E}_h h^2 \leq 2 \max\{1, |\log \xi_f|, |\log \tau_f|\} \cdot r.
\]
Then Theorem 7.16 in (Steinwart & Christmann, 2008) with \( a := 2c_2 \xi_f^{-1} (r/\lambda)^{1/(4\delta')} \) yields that there exist a constant \( c_0 > 0 \) such that
\[
\mathbb{E}_{D \sim P^n} \text{Rad}_D(\mathcal{H}_r, n) \leq c_0 \max\left\{ \xi_f^{3/4 - \delta} \lambda^{-1/4} n^{-1/2}, \right. \\
\left. r^{1/2(1+\delta')} \lambda^{-1/2(1+\delta')} n^{-1/\delta'} \right\}
\]
\[
=: \varphi_n(r).
\]
Simple algebra shows that the condition \( \varphi_n(4r) \leq 2\sqrt{2} \varphi_n(r) \) is satisfied. Since \( 2\sqrt{2} < 4 \), similar arguments show that still hold the statements of the
Peeling Theorem 7.7 in (Steinwart & Christmann, 2008). Consequently, Theorem 7.20 in (Steinwart & Christmann, 2008) can also be applied, if the assumptions on $\varphi_n$ and $r$ are modified to $\varphi_n(4r) \leq 2\sqrt{2}\varphi_n(r)$ and $r \geq \max\{75\varphi_n(r), 1152M^2\tau/n, r^*\}$, respectively. It is easy to verify that the condition $r \geq 75\varphi_n(r)$ is satisfied if

$$r \geq \gamma_n^{-1/(1+2d')},$$

where $\gamma_n$ is a constant, which yields the assertion.

### B.1.3. Proof Related to Section 4.1

**Proof 10 (Proof of Theorem 1)** It is easy to see that $f_{P,E}$ defined by (22) satisfies $f_{P,E} \in E$. Moreover, by Jensen’s inequality and Proposition 1, we have

$$R_{L,P}(f_{P,E}) - R_{L,P}^* = \frac{1}{T} \sum_{t=1}^{T} f_{P,H_t}(f - f)^2 d_P X \leq \frac{1}{T} \sum_{t=1}^{T} (f_{P,H_t}(f - f)^2 d_P X = \frac{1}{T} \sum_{t=1}^{T} R_{L,P}(f_{P,H_t}) - R_{L,P}^* \leq d\alpha c_0^-2 \alpha \frac{h_0\alpha}{h_0\alpha}.$$  

Consequently we get

$$A(\lambda) = \inf_{f \in E} \Omega(h) + R_{L,P}(f) - R_{L,P}^* \leq \Omega(h) + R_{L,P}(f_{P,E}) - R_{L,P}^* \leq c\lambda^{-2+\alpha}.$$  

Then, Theorem 6 implies that with probability $P \otimes P_H$ not less than $1 - 3e^{-r}$, there holds

$$\lambda\Omega(h) + R_{L,D}(f_{D,\lambda}) - R_{L,P}^* \leq 6c\lambda^{-2+\alpha} + 3\gamma_n c_0^-\frac{1}{\alpha} \frac{1}{\alpha} + \frac{1}{\alpha} + 3952M^2\tau/n,$$

where $c$ and $c_0$ are constants defined as in Proposition 1 and Theorem 6. Minimizing the right hand side of (51), we get

$$R_{L,P}(f_{D,\lambda}) - R_{L,P}^* \leq c\lambda^{-2+\alpha},$$

if we choose

$$\lambda_n := n^{-\frac{2+\alpha}{\alpha(1-2d)}} , \qquad h_{0,n} := n^{-\frac{2+1}{1-2d}},$$

where $c\alpha$ is a constant depending on $c, c\alpha, d, M, R$ and $T$. Thus, the assertion is proved.

### B.2. Proof for $f \in C^{1,\alpha}$

#### B.2.1. Proof Related to Section A.2.1

**Proof 11 (Proof of Lemma 5)** For any $x \in \mathbb{R}^d$, we define $b := H(x) - [H(x)] \in \mathbb{R}^d$. Then we have $b' \sim \text{Unif}(0, 1)^d$ according to the definition of $H$. For any $x' \in A_H(x)$, we define

$$z := H(x') - H(x) = (R \cdot S)(x' - x).$$

Then we have

$$x' = x + (R \cdot S)^{-1} z.$$  

Moreover, since

$$[H(x')] = [H(x)],$$

we have $z \in [-b', 1 - b']$.

**Proof 12 (Proof of Proposition 2)** Lemma 1 implies that the excess risk $R_{L,P}(f_{D,E}) - R_{L,P}$ can be controlled by considering the $L_2$-distance $\|f_{D,E} - f\|_{L_2(\mu)}$. According to the generation process, the histogram transforms $\{H_t\}_{t=1}^T$ are i.i.d. Therefore, for any $x \in B_R$, the expected approximation error term can be decomposed as follows:

$$\mathbb{E}_{P}(f_{P,E}(x) - f(x))^2 \leq \mathbb{E}_{P_E}(f_{P,E}(x) - (\mathbb{E}_{P_E}(f_{P,E}(x))))^2 + (\mathbb{E}_{P_E}(f_{P,E}(x)) - f(x))^2 \leq \frac{1}{T} \mathbb{E}_{P_E}(f_{P,H_t}(x) + (\mathbb{E}_{P_E}(f_{P,H_t}(x)) - f(x))^2. \tag{52}$$

In the following, for the simplicity of notations, we drop the subscript of $H_1$ and write $H$ instead of $H_1$ when there is no confusion.

For the first term in (52), the assumption $f \in C^{1,\alpha}$ implies

$$\mathbb{Var}_{P_E}(f_{P,H}(x)) = \mathbb{E}_{P_E}(f_{P,H}(x) - \mathbb{E}_{P_E}(f_{P,H}(x)))^2 \leq \mathbb{E}_{P_E}(f_{P,H}(x) - f(x))^2 \mathbb{E}_{P_E} \left( \frac{1}{\mu(A_H(x))} \int_{A_H(x)} f(x') dx' - f(x) \right)^2 \mathbb{E}_{P_E} \left( \frac{1}{\mu(A_H(x))} \int_{A_H(x)} (f(x') - f(x)) dx' \right)^2 \mathbb{E}_{P_E}(c_{L,diam}(A_H(x))) \leq c_{L,diam}^2 \int_{0}^{1} \text{d}r_0. \tag{53}$$

We now consider the second term in (52). Lemma 5 implies that for any $x' \in A_H(x)$, there exist a random vector $u \sim \text{Unif}[0, 1]^d$ and a vector $v \in [0, 1]^d$ such that

$$x' = x + S^{-1} R^T (-u + v). \tag{54}$$
Therefore, we have
\[
dx' = \det \left( \frac{dx'}{dv} \right) dv = \det \left( \frac{dx + S^{-1}R^T(-u + v)}{dv} \right) dv = \det(RS^{-1}) dv = \left( \prod_{i=1}^{d} h_i \right) dv. \tag{55}
\]
Taking the first-order Taylor expansion of \(f(x')\) at \(x\), we get
\[
f(x') - f(x) = \int_{0}^{1} \left( \nabla f(x + t(x' - x)) \right)^\top (x' - x) dt. \tag{56}
\]
Moreover, we obviously have
\[
\nabla f(x)^\top (x' - x) = \int_{0}^{1} \nabla f(x)^\top (x' - x) dt. \tag{57}
\]
Thus, (56) and (57) imply that for any \(f \in C^{1,\alpha}\), there holds
\[
|f(x') - f(x) - \nabla f(x)^\top (x' - x)| = \left| \int_{0}^{1} \left( \nabla f(x + t(x' - x)) - \nabla f(x) \right)^\top (x' - x) dt \right|
\leq \int_{0}^{1} c_{L}(t)||x' - x||^{2}||x' - x||_{2} dt
\leq c_{L}||x' - x||^{1+\alpha}.
\]
This together with (54) yields
\[
|f(x') - f(x)| \leq \left( f(x') - f(x) \right)^\top S^{-1}R^T(-u + v) \leq c_{L}H_{0}^{1+\alpha},
\]
and consequently there exists a constant \(c_{L} \in [-c_{L}, c_{L}]\) such that
\[
f(x') - f(x) = \nabla f(x)^\top S^{-1}R^T(-u + v) + c_{L}H_{0}^{1+\alpha}. \tag{58}
\]
The definition (14) of \(f_{P,H}(x)\) shows
\[
f_{P,H}(x) = \frac{1}{\mu(A_{H}(x))} \int_{A_{H}(x)} f(x') dx'.
\]
This together with (58) and (55) yields
\[
f_{P,H}(x) - f(x) = \frac{1}{\mu(A_{H}(x))} \int_{A_{H}(x)} \left( f(x') - f(x) \right) dx'
= \prod_{i=1}^{d} h_i \int_{[0,1]^d} \left( \nabla f(x)^\top S^{-1}R^T(-u + v) + c_{L}H_{0}^{1+\alpha} \right) dv
= \left( \int_{[0,1]^d} (-u + v)^\top dv \right) RS^{-1} \nabla f(x) + c_{L}H_{0}^{1+\alpha}
= \left( \frac{1}{2} - u \right)^\top RS^{-1} \nabla f(x) + c_{L}H_{0}^{1+\alpha}. \tag{59}
\]
Since the random variables \((u_i)_{i=1}^{d}\) are independent and identically distributed as \(\text{Unif}[0, 1]\), we have
\[
\mathbb{E}_{P_{H}} \left( \frac{1}{2} - u_i \right) = 0, \quad i = 1, \ldots, d. \tag{60}
\]
Combining (59) with (60), we obtain
\[
\mathbb{E}_{P_{H}} \left( f_{P,H}(x) - f(x) \right) = c_{L}H_{0}^{1+\alpha} \tag{61}
\]
and consequently
\[
\left( \mathbb{E}_{P_{H}} \left( f_{P,H}(1) \right) - f(x) \right)^2 \leq c_{L}^{2}H_{0}^{2(1+\alpha)}. \tag{62}
\]
Combining (52) with (62) and (53), we obtain
\[
\mathbb{E}_{P_{H}} \left( f_{P,E}(x) - f(x) \right)^2 \leq c_{L}^{2}H_{0}^{2(1+\alpha)} + \frac{1}{T} \cdot dc_{L}^{2}H_{0}^{2}. \tag{63}
\]
Taking expectation with respect to \(\mu\), we get
\[
\mathbb{E}_{P_{H}} \left( f_{P,E} - f \right)^2 \leq \frac{c_{L}^{2}H_{0}^{2(1+\alpha)}}{2c_{f}} + \frac{dc_{L}^{2}H_{0}^{2}}{2c_{f}}, \tag{64}
\]
which completes the proof.

**B.2.2. Proof Related to Section A.2.2**

**Proof 13 (Proof of Proposition 3)** Lemma 5 implies that for any \(x' \in A_{H}(x)\), there exist a random vector \(u \sim \text{Unif}[0, 1]^d\) and a vector \(v \in [0, 1]^d\) such that
\[
x' = x + S^{-1}R^T(-u + v).
\]
Then (59) yields
\[
\left( f_{P,H}(x) - f(x) \right)^2 = \left( \left( \frac{1}{2} - u \right)^\top RS^{-1} \nabla f(x) + c_{L}H_{0}^{1+\alpha} \right)^2. \tag{65}
\]
The orthogonality of the rotation matrix \(R\) in Section 3.3 tells us that
\[
\sum_{i=1}^{d} R_{ij}R_{ik} = \begin{cases} 1, & \text{if } j = k, \\ 0, & \text{if } j \neq k \end{cases} \tag{66}
\]
and consequently we have
\[
\sum_{i=1}^{d} \sum_{j \neq k} R_{ij} R_{ik} h_j h_k \cdot \frac{\partial f(x)}{\partial x_j} \cdot \frac{\partial f(x)}{\partial x_k} = \sum_{j \neq k} h_j h_k \cdot \frac{\partial f(x)}{\partial x_j} \cdot \frac{\partial f(x)}{\partial x_k} \sum_{i=1}^{d} R_{ij} R_{ik} = 0.
\]
Since the random variables \((u_i)_{i=1}^{d}\) are independent and identically distributed as \(\text{Unif}[0, 1]\), we have
\[
\mathbb{E}_{P_H} \left( \frac{1}{2} - u_i \right) = 0
\]
and
\[
\mathbb{E}_{P_H} \left( \frac{1}{2} - u_i \right)^2 = \frac{1}{12}.
\]

Then, for all \(x \in B_{R, \sqrt{\sigma P_0}}^+ \cap A_j^f\), (64), (65), (66), and (67) yield
\[
\mathbb{E}_{P_H} \left( \frac{1}{2} - u \right) \top R^{-1} S^{-1} \nabla f(x) \right)^2
\]
\[
= \mathbb{E}_{P_H} \left( \sum_{i=1}^{d} \left( \frac{1}{2} - u_i \right) \sum_{j=1}^{d} R_{ij} h_j \frac{\partial f(x)}{\partial x_j} \right)^2
\]
\[
= \sum_{i=1}^{d} \mathbb{E}_{P_H} \left( \frac{1}{2} - u_i \right)^2 \left( \sum_{j=1}^{d} R_{ij} h_j \frac{\partial f(x)}{\partial x_j} \right)^2
\]
\[
= \frac{1}{12} \mathbb{E}_{P_H} \sum_{i=1}^{d} \sum_{j=1}^{d} R_{ij}^2 h_j^2 \left( \frac{\partial f(x)}{\partial x_j} \right)^2
\]
\[
\geq \frac{d}{12} \epsilon_c^2 \sigma_c \frac{h_0^2}{h_0^2} \geq \frac{d}{12} \epsilon_c^2 \sigma_c^2 \frac{h_0^2}{h_0^2}.
\]
Combining (59) with (68) and using (66), we see that for all \(x \in B_{R, \sqrt{\sigma P_0}}^+ \cap A_j^f\), if
\[
h_0 \leq \left( \frac{\sqrt{d} \epsilon \sigma_c}{4 \sqrt{3} \epsilon L} \right)^2,
\]
then we have
\[
\mathbb{E}_{P_H} (f_{P,H}(x) - f(x))^2 \geq \frac{d}{16} \epsilon_c^2 \sigma_c^2 \frac{h_0^2}{h_0^2}.
\]
where the constant \(c_0\) is as in Assumption 1. Moreover, we have
\[
\mathbb{E}_{P_H} \|f_{P,H} - f\|_2^2 \geq \frac{d}{16} \mu(A_j^f \cap B_{R, \sqrt{\sigma P_0}}^+) \epsilon_c^2 \sigma_c^2 \frac{h_0^2}{h_0^2}.
\]
This completes the proof.
Thus, we proved the assertion.

Then for any

Moreover

Combining (70) with (74), we obtain

Consequently, for all \( x \in B^+_{r,\sqrt{d} \pi_0} \cap A^1_j \) and all \( n \geq N' \), there holds

Moreover

Thus, we proved the assertion.

Proof 15 (Proof of Theorem 7) Recall the error decomposition (25) of single random histogram transform density estimator. Then (69) and (75) yield that for all \( x \in B^+_{R,\sqrt{d} \pi_0} \cap A^1_j \) and all \( n > N_0 \), there holds

By choosing

we obtain

which proves the assertion.

B.2.3. PROOF RELATED TO SECTION A.2.3

Proof 16 (Proof of Theorem 2) Proposition 6 together with Proposition 2 implies

where \( \delta' := 1 - \delta \) and \( \delta := (h_0/c_d)^d \). Choosing

we obtain

This completes the proof.

Proof 17 (Proof of Proposition 5) By (59), we have

Since the random variables \( (u_i)_{i=1}^d \) are independent and identically distributed as Unif[0,1], we have

Consequently we have

\[ E_{P_H} \left( \left( \frac{1}{2} - u_i \right)^3 \right) = E_{P_H} \left( \frac{1}{2} - u_i \right) = 0. \]


Moreover, (68) implies
\[\mathbb{E}_{P_H} \left( \left( \frac{1}{2} - u \right)^T R S^{-1} \nabla f(x) \right)^2 \]
\[= \frac{1}{12} \mathbb{E}_{P_H} \sum_{i=1}^d \sum_{j=1}^d R^2_i h_j^2 \left( \frac{\partial f(x)}{\partial x_j} \right)^2 \leq \frac{d}{12} c_1 h_0^2. \]
Therefore, for any \(x \in B_{\sqrt{n} \sigma}^+ \cap A_1\), we have
\[\mathbb{E}_{P_H} |f_{P,H}(x) - f(x)|^3 \leq \frac{d}{4} c_1 h_0^{1+\alpha} + c_3 h_0^{3(1+\alpha)}. \quad (77)\]

To bound the estimation error, let \(Y := \sum_{i=1}^n 1_{\{X_i \in A_H(x)\}}\) and \(\pi_H\) denote the partition of \(B_R\) induced by \(H\). Then we have \(Y \sim \text{Bin}(n, P(A_H(x)))\) and
\[\mathbb{E}_{P^n} ((f_{D,H}(x) - f_{P,H}(x))^3 | \pi_H) \]
\[= \frac{1}{n^3} P(A_H(x))^3. \]
\[\mathbb{E}_{P^n} \left( \left( \sum_{i=1}^n 1_{X_i \in A_H(x)} - n P(A_H(x)) \right)^3 \pi_H \right) \]
\[= \mathbb{E}_{P^n} ((Y - \mathbb{E}Y)^3). \]
Then the skewness of a binomial random variable implies that for any \(x \in B_{\sqrt{n} \sigma}^+ \cap A_1\), we have
\[\mathbb{E}_{P^n} ((f_{D,H}(x) - f_{P,H}(x))^3 | \pi_H) \]
\[= \frac{P(A_H(x))(1 - P(A_H(x)))(1 - 2P(A_H(x)))}{n^2 P(A_H(x))^3} \]
\[\leq \frac{\bar{\sigma}_f}{n^2 h_0^{2d}} \leq \frac{\bar{\sigma}_f}{c_0^3} n^{-2d} \cdot n^{-2}. \quad (78)\]

Analogously, for any \(x \in B_{\sqrt{n} \sigma}^+ \cap A_1\), there holds
\[\mathbb{E}_{P^n} ((f_{D,H}(x) - f_{P,H}(x))^2 \cdot |f_{P,H}(x) - f(x)|) \]
\[= \mathbb{E}_{P^n} (f_{D,H}(x) - f_{P,H}(x))^2 \cdot \mathbb{E}_{P_H} |f_{P,H}(x) - f(x)| \]
\[\leq \frac{P(A_H(x))(1 - P(A_H(x)))}{n P(A_H(x))^2} \cdot c_L \bar{h}_0^{1+\alpha} \]
\[\leq \frac{c_L^2}{c_0^3} n^{-1} \bar{h}_0^{-d+1+\alpha}. \quad (79)\]

Combining (26) with (77), (78) and (79), we obtain
\[\|f_{D,H} - f\|_{L^3(\mu)}^3 \]
\[\leq \mu(B_{\sqrt{n} \sigma}^+ \cap A_1) \cdot \left( \frac{d}{4} c_1 h_0^{1+\alpha} + c_3 h_0^{3(1+\alpha)} \right) \]
\[+ \frac{\bar{\sigma}_f}{c_0^3} n^{-2d} \bar{h}_0^{-d} + 3 \frac{c_L^2}{c_0^3} n^{-1} \bar{h}_0^{-d+1+\alpha}, \]
which completes the proof.

Proof 18 (Proof of Theorem 3) Lemma 1 together with Theorem 7 and Proposition 5 yields
\[\mathcal{R}_{L,P}(f_{D,H}) - \mathcal{R}_{L,P}^* \geq \frac{\|f_{D,H} - f\|_{L^2(\mu)}^2}{2\mathcal{L}_f} - \frac{\|f_{D,H} - f\|_{L^2(\mu)}^2}{3\mathcal{L}_f} \]
\[\geq \frac{\mathcal{L}_f^2}{2\mathcal{L}_f} - \frac{\mathcal{L}_f^2}{3\mathcal{L}_f} = \mathcal{L}_f. \]
By choosing \(\bar{h}_{0,n} := n^{-\frac{1+\alpha}{2}},\)
we obtain
\[\mathcal{R}_{L,P}(f_{D,H}) - \mathcal{R}_{L,P}^* \geq n^{-\frac{1+\alpha}{2}}, \]
which yields the assertion.

C. Supplementary for Experiments

C.1. Descriptions of Synthetic Datasets

The detailed descriptions are shown in Table 3. In order to give clear visualization of the distributions, we take \(d = 2\) for instance, and give the 3D visualization of the above four types of distributions in Figure 6, where \(x\)-axis and \(y\)-axis represent the 2-dimensional feature space and \(z\)-axis represents the value of the density function.

![Figure 6](image)

(a) Type I  (b) Type II  (c) Type III  (d) Type IV

Figure 6. 3D plots of the synthetic distributions with \(d = 2\).

C.2. Descriptions of Real Datasets

As follows are the datasets alphabetically listed, with the number of instances and features reported after preprocessing.
**GBHT: Gradient Boosting Histogram Transform for Density Estimation**

### Table 3. Descriptions of synthetic datasets.

| Type | True (Marginal) Distribution |
|------|------------------------------|
| I    | $0.4 \cdot \mathcal{N}(e_d, 0.25 \cdot I_d) + 0.6 \cdot \mathcal{N}(-e_d, 0.25 \cdot I_d)$ |
| II   | $f_i := 0.7 \cdot \text{Beta}(2, 10) + 0.3 \cdot \text{Unif}(0.6, 1.0)$ |
| III  | $f_i := 0.5 \cdot \text{Laplace}(0, 0.5) + 0.5 \cdot \text{Unif}(2, 4)$ |
| IV   | $f_i := \text{Exp}(0.5)$ for $i = 1, \ldots, d-1$ and $f_d := \text{Unif}(0, 5)$ |

* For notational simplicity, we denote $e_d := (1, 1, \ldots, 1)$, $e_d' := (1, -1, \ldots, -1)$, $I_d$ as the identity matrix, and $f_i$ as the marginal distribution of the $i$-th dimension. For Types II, III, IV, the marginal distributions of the true density are independent, and the marginal distributions are identical for Types II and III.

### Table 4. Descriptions of Benchmark Datasets

| Datasets | $n$ | $d$ | #outliers(%) | Datasets | $n$ | $d$ | #outliers(%) |
|----------|-----|-----|--------------|----------|-----|-----|--------------|
| arrhythmia | 452 | 274 | 66(15%)      | breastw | 683 | 9  | 239(34.99%) |
| cardio    | 1,831| 21  | 176(9.61%)   | forestcover | 286,048 | 10 | 2747(0.96%) |
| heart     | 267  | 44  | 55(20.60%)   | http     | 567,498 | 3  | 2211(0.39%) |
| ionosphere | 351 | 33  | 126(35.90%)  | letter    | 1,600 | 32 | 100(6.25%)  |
| mammo.    | 11,183| 6   | 260(2.32%)   | mnist     | 7,602 | 100 | 700(9.2%)   |
| mulcross  | 202,144| 64  | 26214(10.00%)| musk      | 3,062 | 166 | 97(3.2%)    |
| optdigits | 5,216| 64  | 150(3%)      | pendigits | 6,870 | 16 | 156(2.27%) |
| pima      | 768  | 8   | 268(34.90%)  | satellite | 6,435 | 36 | 2036(32%)   |
| shuttle   | 49,097| 9   | 3511(7.15%)  | vertebral | 240  | 6  | 30(12.5%)   |
| vowels    | 1,456| 12  | 50(3.43%)    | wbc       | 129  | 13 | 10(7.7%)   |

### Table 5. AUC performance on benchmark datasets

| Datasets | GBHT (Ours) | $k$-NN | iForest | LOF | OCSVM |
|----------|-------------|--------|---------|-----|-------|
| arrhythmia | 0.7952 | 0.8165 | 0.8073 | 0.8130 | 0.7948 |
| breastw   | 0.9872 | 0.9881 | 0.9884 | 0.4676 | 0.9789 |
| heart     | 0.9221 | 0.8744 | 0.9297 | 0.6790 | 0.9473 |
| ionosphere | 0.9360 | 0.8950 | 0.8792 | 0.5778 | 0.6565 |
| letter    | 0.6228 | 0.1908 | 0.2683 | 0.2941 | 0.5000 |
| http      | 0.9970 | 0.2309 | 0.9999 | 0.3675 | 0.9953 |
| mammography | 0.8786 | 0.8527 | 0.8631 | 0.7568 | 0.8721 |
| mnist     | 0.8385 | 0.8591 | 0.8117 | 0.7406 | 0.8216 |
| mulcross  | 1.0000 | 0.0013 | 0.9642 | 0.5848 | 0.9778 |
| musk      | 0.9893 | 0.9367 | 1.0000 | 0.5476 | 0.5281 |
| optdigits | 0.6381 | 0.4292 | 0.7116 | 0.6682 | 0.8966 |
| pendants  | 0.8991 | 0.8607 | 0.9538 | 0.5437 | 0.9607 |
| pima      | 0.6990 | 0.6437 | 0.6796 | 0.6162 | 0.5842 |
| satellite | 0.7223 | 0.7374 | 0.7041 | 0.5701 | 0.7064 |
| shuttle   | 0.9842 | 0.8004 | 0.9974 | 0.6035 | 0.9918 |
| vertebral | 0.5523 | 0.3253 | 0.3585 | 0.5310 | 0.5374 |
| vowels    | 0.9237 | 0.9749 | 0.7588 | 0.9467 | 0.9153 |
| wbc       | 0.9524 | 0.9501 | 0.9412 | 0.9460 | 0.9469 |

* The best results are marked in **bold**, the second best results are marked in underline.

** The last row shows the summation of ranks for each method, which is the lower the better.

- **Adult** is also known as "Census Income" dataset. It contains 48,842 instances with 6 continuous and 8 discrete attributes. Prediction task is to determine whether a person makes over 50K a year.
- **Australian** is an interesting dataset with a good mix of attributes, which contains continuous, nominal...
with both small and large numbers of values. The dataset contains 690 instances with 6 numerical and 9 categorical attributes, mainly concerning credit card applications.

- Breast-cancer is originally for predicting whether a cancer is recurrence event. It contains 675 instances of dimension 11, describing the status of the tumors and the patients.

- Diabetes dataset comprises 768 samples and 9 features. The attributes concern about the medical records of patients, consisting of 8 numerical features and 1 categorical feature.

- Ionosphere is a multivariate dataset for binary classification tasks, attribute to predict is either “good” or “bad”. This radar data was collected by a system in Goose Bay, Labrador. It contains 351 instances of dimension 34.

- Parkinsons dataset is composed of a range of biomedical voice measurements from 31 people, 23 with Parkinson’s disease (PD). It contains 197 instances of dimension 23.

For anomaly detection, we select 20 real datasets from the ODDS library, with various sample sizes and dimensionalities. Details of real-world datasets are shown in Table 4.

C.3. Gradient Boosted Histogram Transform (GBHT) for Anomaly Detection

We conduct numerical experiments to make a comparison between our GBHT and several popular anomaly detection algorithms such as the forest-based Isolation Forest (iForest) (Liu et al., 2008), the distance-based $k$-Nearest Neighbor ($k$-NN) (Ramaswamy et al., 2000) and Local Outlier Factor (LOF) (Breunig et al., 2000), and the kernel-based one-class SVM (OCSVM) (Schölkopf et al., 2001), on 20 real-world benchmark outlier detection datasets from the ODDS library. The detailed descriptions of these datasets can be found in Table 4 in Section C.2 of the supplement. The measure for the performance evaluation is the area under the ROC curve (AUC). For each method, we choose the best AUC performance when parameters go through their parameter grids.

The implementation details are below: For our method, the grid of $s_{\text{min}}$ and $s_{\text{max}} - s_{\text{min}}$ are $\{-3, -2, -1, 0\}$ and $\{0.5, 1, 2, 3\}$, respectively. The number of iterations $T$ is chosen from $\{100, 500\}$. Moreover, we incorporate Nesterov’s descent method (Biau et al., 2019) into our boosting algorithm for accelerating and set shrinkage parameter grid to be $\{0.1, 0.5\}$. For iForest, LOF and OCSVM, we utilized the implementation of scikit-learn. For $k$-NN and LOF, the parameter grid of number of neighbors $k$ is $\{5, 10, 15, \cdots, 45, 50\}$. As for iForest, we set the grid of the number of trees to be $\{100, 500\}$ and sub-sampling size to be 256. For OCSVM, we use RBF kernel with gamma grid $\{0.001, 0.01, \cdots, 1, 10\}$. The experimental results are reported in Table 5.