In this supplementary material, we first prove Theorem 3.2 and then Theorems 3.1 and 3.3.

A Notations and Preliminaries

We use $\sigma$ to denote the ReLU activation function in neural networks, which is $\sigma(x) = \max\{x, 0\}$. Without further indication, $\|\cdot\|$ represents the $L_2$ norm. For any function $g$, let $\|g\|_\infty = \sup_x \|g(x)\|$. We use notation $O(\cdot)$ and $\tilde{O}(\cdot)$ to express the order of function slightly differently, where $O(\cdot)$ omits the universal constant not relying on $d$ while $\tilde{O}(\cdot)$ omits the constant related to $d$. We use $B_d^2(a)$ to denote $L_2$ ball in $\mathbb{R}^d$ with center at $0$ and radius $a$. Let $g_\# \nu$ be the pushforward distribution of $\nu$ by function $g$ in the sense that $g_\# \nu(A) = \nu(g^{-1}(A))$ for any measurable set $A$.

The $r$-covering number of some class $\mathcal{F}$ w.r.t. norm $\|\cdot\|$ is the minimum number of $r$-radius balls needed to cover $\mathcal{F}$, which we denote as $\mathcal{N}(r, \mathcal{F}, \|\cdot\|)$. We denote $\mathcal{N}(r, \mathcal{F}, L_2(P_n))$ as the covering number of $\mathcal{F}$ w.r.t. $L_2(P_n)$, which is defined as $\|f\|_{L_2(P_n)}^2 = \frac{1}{n} \sum_{i=1}^n \|f(X_i)\|^2$ where $X_1, \ldots, X_n$ are the empirical samples. We denote $\mathcal{N}(r, \mathcal{F}, L_\infty(P_n))$ as the covering number of $\mathcal{F}$ w.r.t. $L_\infty(P_n)$, which is defined as $\|f\|_{L_\infty(P_n)} = \max_{1 \leq i \leq n} \|f(X_i)\|$. It is easy to check that
\[
\mathcal{N}(r, \mathcal{F}, L_2(P_n)) \leq \mathcal{N}(r, \mathcal{F}, L_\infty(P_n)) \leq \mathcal{N}(r, \mathcal{F}, \|\cdot\|_\infty).
\]

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B Restriction on the domain of uniformly bounded Lipschitz function class \( \mathcal{F}^1 \)

So far, most of the related works assume that the target distribution \( \mu \) is supported on a compact set, for example \cite{chen2020ips}, and \cite{liang2020ips}. To remove the compact support assumption, we need to assume Assumption 1, i.e., the tails of the target \( \mu \) and the reference \( \nu \) are subexponential. Define \( \mathcal{F}_n^1 := \{ f_{B_n^d \cap ((\sqrt{2} \log n) D)} : f \in \mathcal{F} \} \). In this section, we show that proving Theorem 3.2 is equivalent to establishing the same convergence rate but with the domain restricted function class \( \mathcal{F}_n^1 \) as the evaluation class.

Under Assumption 1 and by the Markov inequality, we have

\[
P_\nu(\|z\| > \log n) \leq \frac{\mathbb{E}_\nu \|z\| 1_{\|z\| > \log n}}{\log n} = O(n^{-\frac{(\log n)^d}{d}} / \log n) \tag{B.1}
\]

The Dudley distance between latent joint distribution \( \hat{\nu} \) and data joint distribution \( \hat{\mu} \) is defined as

\[
d_{\mathcal{F}^1}(\hat{\nu}, \hat{\mu}) = \sup_{f \in \mathcal{F}^1} \mathbb{E} f(\hat{g}(z), z) - \mathbb{E} f(x, \hat{e}(x)) \tag{B.2}
\]

The first term above can be decomposed as

\[
\mathbb{E} f(\hat{g}(z), z) = \mathbb{E} f(\hat{g}(z), z) 1_{\|z\| \leq \log n} + \mathbb{E} f(\hat{g}(z), z) 1_{\|z\| > \log n} \tag{B.3}
\]

For any \( f \in \mathcal{F}^1 \) and fixed point \( z_0 \) such that \( \|z_0\| \leq \log n \), due to the Lipschitzness of \( f \), the second term above satisfies

\[
|\mathbb{E} f(\hat{g}(z), z) 1_{\|z\| > \log n}| \leq |\mathbb{E} f(\hat{g}(z), z) 1_{\|z\| > \log n} - \mathbb{E} f(\hat{g}(z_0), z_0) 1_{\|z\| > \log n}| + |\mathbb{E} f(\hat{g}(z_0), z_0) 1_{\|z\| > \log n}|
\]

\[
\leq \mathbb{E} \|\hat{g}(z) - \hat{g}(z_0)\| 1_{\|z\| > \log n} + \mathbb{E} \mathbb{P}_\nu(\|z\| > \log n) + B \mathbb{P}_\nu(\|z\| > \log n)
\]

\[
\leq 2(\log n) \mathbb{P}_\nu(\|z\| > \log n) + \mathbb{E} \|z - z_0\| 1_{\|z\| > \log n} + B \mathbb{P}_\nu(\|z\| > \log n)
\]

\[
= O(n^{-\frac{(\log n)^d}{d}})
\]

where the second inequality is due to lipschitzness and boundedness of \( f \), and the last inequality is due to Assumption 1 and the boundedness of \( \hat{g} \). In the first term in (B.3), \( f \) only acts on the increasing \( L_2 \) ball \( B_n^d((\sqrt{2} \log n) D) \) because of Condition 1 and the indicator function \( 1_{\|z\| \leq \log n} \). Similarly, we can apply the same procedure to the second term in (B.2). Therefore, it is still an equivalent problem if we restrict the domain of \( \mathcal{F}^1 \) on \( B_n^d((\sqrt{2} \log n) D) \). Hence, in order to prove the estimation error rate in Theorem 3.2, we only need to show that for the restricted evaluation function class \( \mathcal{F}_n^1 \), we have

\[
\mathbb{E} d_{\mathcal{F}_n^1}(\hat{\nu}, \hat{\mu}) \leq C_0 \sqrt{dn^{-\frac{1}{d+1}} (\log n)^{1+\frac{1}{d+1}}} \land C_{d} n^{-\frac{1}{d+1}} \log n
\]

Due to this fact, to keep notation simple, we are going to denote \( \mathcal{F}_n^1 \) as \( \mathcal{F}^1 \) in the following sections.

Remark 1. The restriction on \( \mathcal{F}^1 \) is technically necessary for calculating the covering number of \( \mathcal{F}^1 \) later we will see the use of it when bounding the stochastic error \( \mathcal{E}_3 \) and \( \mathcal{E}_4 \) below.

C Stochastic errors

C.1 Bounding \( \mathcal{E}_3 \) and \( \mathcal{E}_4 \)

The stochastic errors \( \mathcal{E}_3 \) and \( \mathcal{E}_4 \) quantify how close the empirical distributions and the true latent joint distribution (data joint distribution) are with the Lipschitz class \( \mathcal{F}^1 \) as the evaluation class under IPM. We apply the results in Lemma C.1 to bound \( \mathcal{E}_3 \) and \( \mathcal{E}_4 \). We introduce two methods to bound \( \max \{ \mathcal{E}_3, \mathcal{E}_4 \} \), which gives two different upper bounds for \( \max \{ \mathcal{E}_3, \mathcal{E}_4 \} \). They both utilize the following lemma, which we shall prove later. More detailed description about the refined Dudley inequality can be found in \cite{Srebro2010} and \cite{Schreuder2020}.

2
Lemma C.1 (Refined Dudley Inequality). For a symmetric function class \( \mathcal{F} \) with 
\[
\sup_{f \in \mathcal{F}} \|f\|_\infty \leq M,
\]
we have
\[
\mathbb{E}[d_\mathcal{F}(\hat{\mu}_n, \mu)] \leq \inf_{0 < \delta < M} \left( 4\delta + \frac{12}{\sqrt{n}} \int_{\delta}^{M} \sqrt{\log N(\epsilon, \mathcal{F}, \|\cdot\|_{\infty})} \, d\epsilon \right).
\]

Remark 2. The original Dudley inequality (Dudley [1967]; Van der Vaart and Wellner [1996]) suffers from the problem that if the covering number \( N(\epsilon, \mathcal{F}, \|\cdot\|_{\infty}) \) increases too fast as \( \epsilon \) goes to 0, then the upper bound can be infinite. The improved Dudley inequality circumvents this problem by only allowing \( \epsilon \) to integrate from \( \delta > 0 \), which also indicates that \( \mathbb{E} \mathcal{E}_3 \) scales with the covering number \( N(\epsilon, \mathcal{F}, \|\cdot\|_{\infty}) \).

C.1.1 The first method (explicit constant)

The first method provides an explicit constant depending on \( d \) at the expense of the higher order of \( \log n \) in the upper bounds. It utilizes the next lemma (Gottlieb et al. [2013], Lemma 6), which turns the problem of bounding the covering number of a Lipschitz function class into the one bounding the covering number of the domain defined for the function class.

Lemma C.2 (Gottlieb et al. [2013]). Let \( \mathcal{F}^L \) be the collection of \( L \)-Lipschitz functions mapping the metric space \( (X, \rho) \) to \([0, 1] \). Then the covering number of \( \mathcal{F}^L \) can be estimated in terms of the covering number of \( X \) with respect to \( \rho \) as follows.

\[
N(\epsilon, \mathcal{F}^L, \|\cdot\|_{\infty}) \leq (\frac{8}{\epsilon})^{N(\epsilon/4, L, X, \rho)}.
\]

Now we apply Lemma C.2 to bound the covering number for the 1-Lipschitz class \( N(\epsilon, \mathcal{F}^1, \|\cdot\|_{\infty}) \) by bounding the covering number for its domain \( N(\epsilon, B_2^{d+1}(\sqrt{2} \log n), \|\cdot\|_2) \). Define a new function class \( \mathcal{F}^\frac{1}{d+1} \) as

\[
\mathcal{F}^\frac{1}{d+1} := \{ \frac{f + B}{2B} : f \in \mathcal{F}^1 \}.
\]

Recall that \( \mathcal{F}^1 \) is restricted on \( B_2^{d+1}(\sqrt{2} \log n) \). Obviously, \( \mathcal{F}^\frac{1}{d+1} \) is a \( \frac{1}{d+1} \)-Lipschitz function class:

\[
\mathcal{F}^\frac{1}{d+1} : B_2^{d+1}(\sqrt{2} \log n) \rightarrow [0, 1].
\]

A direct application of Lemma C.2 shows that

\[
N(\epsilon, \mathcal{F}^\frac{1}{d+1}, \|\cdot\|_{\infty}) \leq (\frac{8}{\epsilon})^{N(\epsilon B/4, B_2^{d+1}(\sqrt{2} \log n), \|\cdot\|_2)}.
\]

(C.1)

By the definition of \( \mathcal{F}^\frac{1}{d+1} \), the covering numbers satisfy

\[
N(2B\epsilon, \mathcal{F}^1, \|\cdot\|_{\infty}) = N(\epsilon, \mathcal{F}^\frac{1}{d+1}, \|\cdot\|_{\infty}).
\]

(C.2)

Note that \( B_2^{d+1}(\sqrt{2} \log n) \) is a subset of \([-\sqrt{2} \log n, \sqrt{2} \log n]^d \), and \([-\sqrt{2} \log n, \sqrt{2} \log n]^d \) can be covered with finite \( \epsilon \)-balls in \( \mathbb{R}^d \) that cover the small hypercube with side length \( 2\epsilon/\sqrt{d} \). It follows that

\[
N(\epsilon, B_2^{d+1}(\sqrt{2} \log n), \|\cdot\|_2) \leq \left( \frac{\sqrt{2(d+1) \log n}}{\epsilon} \right)^{d+1}.
\]

(C.3)

Combining (C.1), (C.2) and (C.3), we obtain an upper bound for the covering number of the 1-Lipschitz class \( \mathcal{F}^1 \)

\[
\log N(\epsilon, \mathcal{F}^1, \|\cdot\|_{\infty}) \leq \left( \frac{8 \sqrt{2(d+1) \log n}}{\epsilon} \right)^{d+1} \log \frac{16B}{\epsilon}.
\]

(C.4)

With the upper bound for the covering entropy in (C.4), a direct application of Lemma C.1 (see Section E for details) by taking \( \delta = \sqrt{2(d+1) \log n} \) leads to

\[
\max \{ \mathbb{E} \mathcal{E}_3, \mathbb{E} \mathcal{E}_4 \} = O \left( \sqrt{dn} \log \left( \sqrt{dn} \right)^{d+1} \log \frac{16B}{\epsilon} \right).
\]

(C.5)
C.1.2 The second method (better order of $\log n$)

We now consider the second method that leads to a better order for the $\log n$ term in the upper bound at the expense of explicitness of the constant related to $d$. The next lemma directly provides an upper bound for the covering number of Lipschitz class but with an implicit constant related to $d$. It is a straightforward corollary of Van der Vaart and Wellner [1996, Theorem 2.7.1].

Lemma C.3. Let $\mathcal{X}$ be a bounded, convex subset of $\mathbb{R}^d$ with nonempty interior. There exists a constant $c_d$ depending only on $d$ such that

$$
\log \mathcal{N}(\epsilon, \mathcal{F}^1(\mathcal{X}), \| \cdot \|_\infty) \leq c_d \lambda(\mathcal{X}^1) \left( \frac{1}{\epsilon} \right)^d
$$

for every $\epsilon > 0$, where $\mathcal{F}^1(\mathcal{X})$ is the 1-Lipschitz function class defined on $\mathcal{X}$, and $\lambda(\mathcal{X}^1)$ is the Lebesgue measure of the set $\{ x : \| x - \mathcal{X} \| < 1 \}$.

Applying Lemmas C.1 and C.3 (see Section C for details) by taking $\delta = n^{-\frac{1}{d+1}} \log n$ yields

$$
\max \{ \mathbb{E} \mathcal{E}_3, \mathbb{E} \mathcal{E}_4 \} = O \left( C_d n^{-\frac{1}{d+1}} \log n \right),
$$

where $C_d$ is some constant depending on $d$. Combining (C.6) and (C.7), we get

$$
\max \{ \mathbb{E} \mathcal{E}_3, \mathbb{E} \mathcal{E}_4 \} = O \left( C_d n^{-\frac{1}{d+1}} \log n \wedge \sqrt{d} n^{-\frac{1}{d+1}} (\log n)^{1+\frac{1}{d+1}} \right).
$$

Remark 3. Here, we have a tradeoff between the logarithmic factor $\log n$ and the explicitness of the constant depending on $d$. If we want an explicit constant depending on $d$, then we have the factor $(\log n)^{1+\frac{1}{d+1}}$ in the upper bound. Later we will see that $\mathbb{E} \mathcal{E}_3$ and $\mathbb{E} \mathcal{E}_4$ are the dominating terms in the four error terms, hence the explicitness of the corresponding constant becomes important. Therefore, we list two different methods here to bound $\mathbb{E} \mathcal{E}_3$ and $\mathbb{E} \mathcal{E}_4$.

C.2 Combination of the four error terms

With all the upper bounds for the four different error terms obtained above, next we consider $\mathcal{E}_1$-$\mathcal{E}_4$ simultaneously to obtain an overall convergence rate. First, recall how we bound $\mathcal{E}_1$ and $\mathcal{E}_4$. With Lemma 4.2, we have

$$
\mathcal{E}_1 = O \left( \sqrt{d} (W_1 L_1)^{-\frac{1}{d+1}} \log n \right).
$$

To control $\mathcal{E}_1$ while keeping the architecture of discriminator class $\mathcal{F}_{NN}$ as small as possible, we let $W_1 L_1 = [\sqrt{n}]$, so that $\mathcal{E}_1 = O \left( \sqrt{d} n^{-\frac{1}{d+1}} \log n \right)$ dominated by $\mathcal{E}_3$ and $\mathcal{E}_4$.

By Theorem 4.3 we can choose the architectures of generator and encoder classes accordingly to perfectly control $\mathcal{E}_2$, i.e. $\mathcal{E}_2 = 0$.

We note that because we imposed Condition [1] on both generator and encoder classes, Theorem 4.3 can not be applied if we have some $\| x_i \|$ or $\| z_i \|$ greater than $\log n$, in which case $\mathcal{E}_2$ can not be perfectly controlled. But we can still handle this case by considering the probability of the bad set.

Under Condition [1] on the nice set $A := \{ \max_{1 \leq i \leq n} \| x_i \| \leq \log n \} \cap \{ \max_{1 \leq i \leq n} \| z_i \| \leq \log n \}$, we have $\mathcal{E}_2 = 0$. Probability of the nice set $A$ has the following lower bound.

$$
P(A) = P_\mu(\| x_i \| \leq \log n)^n \cdot P_\nu(\| z_i \| \leq \log n)^n
$$

$$
\geq (1 - C n^{-\frac{(\log n)^{d'}}{d}})^{2n}, \quad \text{for some constant } C > 0 \text{ by Assumption [1]}
$$

$$
\geq 1 - C n^{-\frac{(\log n)^{d'}}{d}} \cdot (2n), \quad \text{for large } n.
$$

The bad set $A^c$ is where $\mathcal{E}_2 > 0$, which has the probability upper bound as follows.

$$
P(A^c) \leq C n^{-\frac{(\log n)^{d'}}{d}} \cdot (2n)
$$

$$
= O \left( n^{-\frac{(\log n)^{d'}}{d'}} \right), \quad \text{for any } \delta' < \delta.
$$
In Assumption 1, the \((\log n)^d\) factor was to make the tail of the target \(\mu\) strictly subexponential, which leads to \(P(A^c) \to 0\), while the exponential tail or heavier will cause the undesired result \(P(A^c) \to 1\).

Now we are ready to obtain the desired result in Theorem 3.2. The nice set \(A = \{\max_{1 \leq i \leq n} \|x_i\| \leq \log n\} \cap \{\max_{1 \leq i \leq n} \|z_i\| \leq \log n\}\) is where \(E_2 = 0\). By combining the results discussed above, we have

\[
E_d F_1(\hat{\nu}, \hat{\mu}) = 2E_1 + E_2 \mathbb{1}_A + E_3 + E_4
\]

\[
\leq O \left( \sqrt{dn} - \frac{1}{\pi} \log n + 2BP_{\mu}(A^c) + \sqrt{dn} - \frac{1}{\pi} (\log n)^{1 + \frac{1}{d+1}} \wedge C_d n - \frac{1}{\pi} \log n \right)
\]

\[
= O \left( \sqrt{dn} - \frac{1}{\pi} (\log n)^{1 + \frac{1}{d+1}} \wedge C_d n - \frac{1}{\pi} \log n \right)
\]

which completes the proof of Theorem 3.2.

D Proof of Inequality (4.2)

For ease of reference, we restate inequality (4.2) as the following lemma.

**Lemma 4.2.** For any symmetric function classes \(F\) and \(H\), denote the approximation error \(E(H, F)\) as

\[
E(H, F) := \sup_{h \in H} \inf_{f \in F} \|h - f\|_\infty,
\]

then for any probability distributions \(\mu\) and \(\nu\),

\[
d_H(\mu, \nu) - d_F(\mu, \nu) \leq 2E(H, F).
\]

**Proof of Lemma 4.2.** By the definition of supremum, for any \(\epsilon > 0\), there exists \(h_\epsilon \in H\) such that

\[
d_H(\mu, \nu) := \sup_{h \in H} [E_\mu h - E_\nu h]
\]

\[
\leq E_\mu h_\epsilon - E_\nu h_\epsilon + \epsilon
\]

\[
= \inf_{f \in F} [E_\mu (h_\epsilon - f) - E_\nu (h_\epsilon - f) + E_\mu (f) - E_\nu (f)] + \epsilon
\]

\[
\leq 2 \inf_{f \in F} \|h_\epsilon - f\|_\infty + d_F(\mu, \nu) + \epsilon
\]

\[
\leq 2E(H, F) + d_F(\mu, \nu) + \epsilon,
\]

where the last line is due to the definition of \(E(H, F)\). \(\square\)

It is easy to check that if we replace \(d_H(\mu, \nu)\) by \(\hat{d}_H(\mu, \nu) := \sup_{h \in H} [\hat{E}_\mu h - \hat{E}_\nu h]\), Lemma 4.2 still holds.

E Bounding \(E E_3\) and \(E E_4\)

E.1 Method One

With the upper bound for the covering entropy (C.4), i.e.

\[
\log \mathcal{N}(\epsilon, F^1, \|\cdot\|_\infty) \leq \left( \frac{8 \sqrt{2(d + 1) \log n}}{\epsilon} \right)^{d+1} \log \frac{16B}{\epsilon}
\]
and \( \delta = 8\sqrt{2(d + 1)n^{-\frac{d+1}{2}}} (\log n)^{1+\frac{d+1}{2}} \), applying Lemma \( \text{C.1} \) we have

\[
\mathbb{E} \mathcal{E}_3 = O \left( \delta + n^{-\frac{1}{2}} \int_\delta^B \left( \frac{8\sqrt{2(d + 1) \log n}}{\epsilon} \right)^\frac{d+1}{2} \left( \frac{\log \frac{16B}{\epsilon}}{d+1} \right)^\frac{1}{2} \right) \\
= O \left( \delta + n^{-\frac{1}{2}} \left( 8\sqrt{2(d + 1) \log n} \right)^\frac{d+1}{2} \left( \delta \right)^{\frac{d+1}{2}} \right) \\
= O \left( \sqrt{d} n^{-\frac{d+1}{2}} (\log n)^{1+\frac{d+1}{2}} + n^{-\frac{1}{2}} (\log n)^{1+\frac{d+1}{2}} \right) \\
= O \left( \sqrt{d} n^{-\frac{d+1}{2}} (\log n)^{1+\frac{d+1}{2}} \right),
\]

where the second equality is due to

\[
\log \frac{16B}{\epsilon} = O \left( \log \frac{1}{\epsilon} \right) = O \left( \log \frac{n^{\frac{\pi}{2d}}} {8\sqrt{2(d + 1)(\log n)^{1+\frac{d+1}{2}}} \right) \\
= O \left( \log n^{\frac{1}{\pi d}} \right),
\]

and the third equality follows from simple algebra.

**E.2 Method Two**

By Lemma \( \text{C.3} \) we have

\[
\log \mathcal{N}(\epsilon, \mathcal{F}^1, \| \cdot \|_{\infty}) \leq c_d \left( \frac{\log n}{\epsilon} \right)^{d+1}.
\]

Taking \( \delta = n^{-\frac{\pi}{2d}} \log n \) and applying Lemma \( \text{C.1} \) we obtain

\[
\mathbb{E} \mathcal{E}_3 = O \left( \delta + \left( \frac{c_d}{n} \right)^{\frac{1}{2}} (\log n)^{\frac{d+1}{2}} \int_\delta^M \left( \frac{1}{\epsilon} \right)^{\frac{d+1}{2}} \right) \\
= \tilde{O} \left( \delta + n^{-\frac{1}{2}} (\log n)^{\frac{d+1}{2}} \delta^{\frac{d+1}{2}} \right) \\
= \tilde{O} \left( n^{-\frac{\pi}{2d}} \log n \right),
\]

where \( \tilde{O}(\cdot) \) omitted the constant related to \( d \).

**F Proof of Lemma \( \text{C.1} \)**

For completeness we provide a proof of the refined Dudley’s inequality in Lemma \( \text{C.1} \). We apply the standard symmetrization and chaining technics in the proof, see, for example, Van der Vaart and Wellner (1996).

**Proof.** Let \( Y_1, \ldots, Y_n \) be random samples from \( \mu \) which are independent of \( X_i \)’s. Then we have

\[
\mathbb{E} d_F(\hat{\mu}_n, \mu) = \mathbb{E} \sup_{f \in F} \left[ \frac{1}{n} \sum_{i=1}^n f(X_i) - \mathbb{E} f(X_i) \right] \\
= \mathbb{E} \sup_{f \in F} \left[ \frac{1}{n} \sum_{i=1}^n f(X_i) - \frac{1}{n} \sum_{i=1}^n f(Y_i) \right] \\
\leq \mathbb{E} \sup_{f \in F} \left[ \frac{1}{n} \sum_{i=1}^n f(X_i) - \frac{1}{n} \sum_{i=1}^n f(Y_i) \right] \\
= \mathbb{E} \sup_{f \in F} \left[ \frac{1}{n} \sum_{i=1}^n \epsilon_i (f(X_i) - f(Y_i)) \right] \\
\leq 2\mathbb{E} \mathcal{R}_n(F)
\]
where the first inequality is due to Jensen inequality, and the third equality is because that \((f(X_i) - f(Y_i))\) has symmetric distribution.

Let \(\alpha_0 = M\) and for any \(j \in \mathbb{N}_+\) let \(\alpha_j = 2^{-j} M\). For each \(j\), let \(T_j\) be a \(\alpha_j\)-cover of \(\mathcal{F}\) w.r.t. \(L_2(P_n)\) such that \(|T_j| = \mathcal{N}(\alpha_j, F, L_2(P_n))\). For each \(f \in \mathcal{F}\) and \(j\), pick a function \(\hat{f}_j \in T_j\) such that \(\|\hat{f}_j - f\|_{L_2(P_n)} < \alpha_j\). Let \(\hat{f}_0 = 0\) and for any \(N\), we can express \(f\) by chaining as

\[
f = f - \hat{f}_N + \sum_{i=1}^N (\hat{f}_i - \hat{f}_{i-1}).
\]

Hence for any \(N\), we can express the empirical Rademacher complexity as

\[
\hat{\mathcal{R}}_n(\mathcal{F}) = \frac{1}{n} \mathbb{E}_\varepsilon \sup_{f \in \mathcal{F}} \sum_{i=1}^n \varepsilon_i \left( f(X_i) - \hat{f}_N(X_i) + \sum_{j=1}^N (\hat{f}_j(X_i) - \hat{f}_{j-1}(X_i)) \right)
\]

\[
\leq \frac{1}{n} \mathbb{E}_\varepsilon \sup_{f \in \mathcal{F}} \sum_{i=1}^n \varepsilon_i \left( f(X_i) - \hat{f}_N(X_i) \right) + \sum_{i=1}^n \frac{1}{n} \mathbb{E}_\varepsilon \sup_{f \in \mathcal{F}} \sum_{j=1}^N \varepsilon_i \left( \hat{f}_j(X_i) - \hat{f}_{j-1}(X_i) \right)
\]

\[
\leq \|\varepsilon\|_{L_2(P_n)} \sup_{f \in \mathcal{F}} \| f - \hat{f}_N \|_{L_2(P_n)} + \sum_{i=1}^n \frac{1}{n} \mathbb{E}_\varepsilon \sup_{f \in \mathcal{F}} \sum_{j=1}^N \varepsilon_i \left( \hat{f}_j(X_i) - \hat{f}_{j-1}(X_i) \right)
\]

\[
= \alpha_N + \sum_{i=1}^n \frac{1}{n} \mathbb{E}_\varepsilon \sup_{f \in \mathcal{F}} \sum_{j=1}^N \varepsilon_i \left( \hat{f}_j(X_i) - \hat{f}_{j-1}(X_i) \right),
\]

where \(\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)\) and the second-to-last inequality is due to Cauchy–Schwarz. Now the second term is the summation of empirical Rademacher complexity w.r.t. the function classes \(\{f' - f'' : f'' \in T_j, f'' \in T_{j-1}\}, j = 1, \ldots, N\). Note that

\[
\|\hat{f}_j - \hat{f}_{j-1}\|_{L_2(P_n)}^2 \leq \left( \|\hat{f}_j - f\|_{L_2(P_n)} + \|f - \hat{f}_{j-1}\|_{L_2(P_n)} \right)^2
\]

\[
\leq (\alpha_j + \alpha_{j-1})^2
\]

\[
= 3\alpha_j^2.
\]

Massart’s lemma ([Mohri et al., 2018] Theorem 3.7) states that if for any finite function class \(\mathcal{F}\), \(\sup_{f \in \mathcal{F}} \| f \|_{L_2(P_n)} \leq M\), then we have

\[
\hat{\mathcal{R}}_n(\mathcal{F}) \leq \sqrt{\frac{2M^2 \log(|\mathcal{F}|)}{n}}.
\]

Applying Massart’s lemma to the function classes \(\{f' - f'' : f' \in T_j, f'' \in T_{j-1}\}, j = 1, \ldots, N\), we get that for any \(N\),

\[
\hat{\mathcal{R}}_n(\mathcal{F}) \leq \alpha_N + \sum_{j=1}^N 3\alpha_j \sqrt{\frac{2 \log(|T_j| \cdot |T_{j-1}|)}{n}}
\]

\[
\leq \alpha_N + 6 \sum_{j=1}^N \alpha_j \sqrt{\frac{\log(|T_j|)}{n}}
\]

\[
\leq \alpha_N + 12 \sum_{j=1}^N (\alpha_j - \alpha_{j+1}) \sqrt{\frac{\log \mathcal{N}(\alpha_j, \mathcal{F}, L_2(P_n))}{n}}
\]

\[
\leq \alpha_N + 12 \int_{\alpha_{N+1}}^{\alpha_0} \sqrt{\frac{\log \mathcal{N}(r, \mathcal{F}, L_2(P_n))}{n}} \, dr,
\]

where the third inequality is due to \(2(\alpha_j - \alpha_{j+1}) = \alpha_j\). Now for any small \(\delta > 0\) we can choose \(N\) such that \(\alpha_{N+1} \leq \delta < \alpha_N\). Hence,

\[
\hat{\mathcal{R}}_n(\mathcal{F}) \leq 2\delta + 12 \int_{\delta/2}^{\delta} \sqrt{\frac{\log \mathcal{N}(r, \mathcal{F}, L_2(P_n))}{n}} \, dr.
\]
Since $\delta > 0$ is arbitrary, we can take inf w.r.t. $\delta$ to get
\[
\hat{R}_n(\mathcal{F}) \leq \inf_{0<\delta<M} \left( 4\delta + 12 \int_{\delta}^{M} \frac{\log N(r, \mathcal{F}, L_2(P_n))}{n} dr \right).
\]

The result follows due to the fact that
\[
N(r, \mathcal{F}, L_2(P_n)) \leq N(\epsilon, \mathcal{F}, L_\infty(P_n)) \leq N(\epsilon, \mathcal{F}, \|\cdot\|_{\infty}).
\]

\section{G Proof of Theorem 3.1}

Proof. Taking $W_1L_1 = \lfloor \sqrt{n} \rfloor$, Shen et al. (2019, Theorem 4.3) gives rise to $E_1 = O(\sqrt{dn^-\frac{d+1}{d+1}})$. The range of $g$ and $e$ covers the supports of $\mu$ and $\nu$, respectively, hence Theorem 3.1 leads to $E_2 = 0$. By Lemma C.2, we have
\[
\log N(\epsilon, \mathcal{F}^{-1}, \|\cdot\|_{\infty}) \leq \left( \frac{8\sqrt{2(d+1)M}}{\epsilon} \right)^{d+1} \log \frac{16B}{\epsilon}.
\]

Now following the same procedure as in Section E by taking $\delta = 8\sqrt{2(d+1)n}^{-\frac{d+1}{d+1}} (\log n)^{\frac{d+1}{d+1}}$, we have
\[
\max \{ E_3, E_4 \} = O \left( \sqrt{dn^-\frac{d+1}{d+1}} (\log n)^{\frac{d+1}{d+1}} \right).
\]

At last, we consider all four error terms simultaneously.
\[
E_{d_{x^+}}(\nu, \tilde{\mu}) \leq E_1 + E_2 + E_3 + E_4 = O \left( \sqrt{dn^-\frac{d+1}{d+1}} (\log n)^{\frac{d+1}{d+1}} \right).
\]

\section{H Proof of Theorem 3.3}

Following the same proof as Theorem 4.3, we have the following theorem.

**Theorem H.1.** Suppose $\nu$ supported on $\mathbb{R}^k$ and $\mu$ supported on $\mathbb{R}^d$ are both absolutely continuous w.r.t. Lebesgue measure, and $z_i$'s and $x_i$'s are i.i.d. samples from $\nu$ and $\mu$, respectively for $1 \leq i \leq n$. Then there exist generator and encoder neural network functions $g : \mathbb{R}^k \to \mathbb{R}^d$ and $e \in \mathbb{R}^d \to \mathbb{R}^k$ such that $g$ and $e$ are inverse bijections of each other between $\{ z_i : 1 \leq i \leq n \}$ and $\{ x_i : 1 \leq i \leq n \}$. Moreover, such neural network functions $g$ and $e$ can be obtained by properly specifying $W_2L_2 = c_2dn$ and $W_2L_3 = c_3kn$ for some constant $12 \leq c_2, c_3 \leq 384$.

Since $\mu$ and $\nu$ are absolutely continuous by assumption, they are also absolutely continuous in any one dimension. Hence the proof reduces to the one-dimensional case.

\section{I Additional Lemma}

Denote $\mathcal{S}^d(z_0, \ldots, z_{N+1})$ as the set of all continuous piecewise linear functions $f : \mathbb{R} \to \mathbb{R}^d$ which have breakpoints only at $z_0 < z_1 < \cdots < z_N < z_{N+1}$ and are constant on $(-\infty, z_0)$ and $(z_{N+1}, \infty)$. The following lemma is a result in Yang et al. (2021).

**Lemma I.1.** Suppose that $W \geq 7d + 1$, $L \geq 2$ and $N \leq (W-d-1)\left\lfloor \frac{W-d-1}{6d} \right\rfloor \left\lfloor \frac{L}{2} \right\rfloor$. Then for any $z_0 < z_1 < \cdots < z_N < z_{N+1}$, $\mathcal{S}^d(z_0, \ldots, z_{N+1})$ can be represented by a ReLU FNNs with width and depth no larger than $W$ and $L$, respectively.

This result indicates that the expressive capacity of ReLU FNNs for piecewise linear functions. If we choose $N = (W-d-1)\left\lfloor \frac{W-d-1}{6d} \right\rfloor \left\lfloor \frac{L}{2} \right\rfloor$, a simple calculation shows $eW^2L/d \leq N \leq CW^2L/d$ with $c = 1/384$ and $C = 1/12$. This means when the number of breakpoints are moderate compared with the network structure, such piecewise linear functions are expressible by feedforward ReLU networks.
References


