Supplementary Materials for "Conditional Diffusion Models are Minimax-Optimal and Manifold-Adaptive for Conditional Distribution Estimation"

Notation: We adopt the notations in the manuscript, and further introduce the following additional notations for the technical proofs. For neural network class $\Phi(H, W, R, B, V)$, we write $\Phi(H, W, R, B) = \Phi(H, W, R, B, \infty)$ if there is no constraint on the function norm. For any $U \subset \mathcal{M}$, we denote $U_X = \{x \in \mathcal{M}_X$: there exists $y \in \mathcal{M}_y$ so that $(x, y) \in U\}$, $U_{Y|x} = \{y \in \mathcal{M}_{Y|x} : (x, y) \subset U\}$ and $U_Y = \bigcup_{x \in U_X} U_{Y|x}$. For any measure ν on $\mathcal{Z}$ and map $G : \mathcal{Z} \to \mathcal{X}$, the pushforward measure $\mu = G_{\#}\nu$ is defined as the unique measure on $\mathcal{X}$ such that $\mu(A) = \nu\big(G^{-1}(A)\big)$ holds for any measurable set A on $\mathcal{X}$. We use $N(\mathcal{F}, \widetilde{d}, \epsilon)$ to denote the ϵ-covering number of function space $\mathcal{F}$ with respect to pseudo-metric $\widetilde{d}$. For any positive integer m, we use the shorthand $[m] := \{1, \cdots, m\}$. For $\alpha \in \mathbb{R}$, the floor and ceiling functions are denoted by $\lfloor \alpha \rfloor$ and $\lceil \alpha \rceil$, indicating rounding α to the next smaller and larger integer. For two sequences $\{a_n\}$ and $\{b_n\}$, we use the notation $a_n \lesssim b_n$ and $a_n \gtrsim b_n$ to mean $a_n \leq C b_n$ and $a_n \geq C b_n$, respectively, for some constant $C > 0$ independent of n. In addition, $a_n \asymp b_n$ means that both $a_n \lesssim b_n$ and $a_n \gtrsim b_n$ hold. We use $\|\cdot\|_\infty$ to denote the usual vector ℓ_∞ norm (i,e., for $x = (x_1, x_2, \cdots, x_d)$, $\|x\|_\infty = \max_i |x_i|$) and reserve $\|\cdot\|$ for the vector ℓ_2 norm. For a vector $x \in \mathbb{R}^d$, we use x_i to denote its ith element. For a multi-index $j = (j_1, \cdots, j_d) \in \mathbb{N}_0^d = \{(j_1, \cdots, j_d) \,|\, \forall i \in [d], j_i \in \mathbb{N}_0\}$, we define $|j| = \sum_{i=1}^d j_i$ and $j! = \prod_{i=1}^d j_i!$. For two vectors $x, y \in \mathbb{R}^d$, we use $(x - y)^j$ to denote $\prod_{i=1}^d (x_i - y_i)^{j_i}$. For a multivariate function $f : \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \to \mathbb{R}$ and multi-indexes $j_1 \in \mathbb{N}_0^{d_1}$, $j_2 \in \mathbb{N}_0^{d_2}$ we use $f^{(j_1, j_2)}$ to denote its mixed partial derivative $\frac{\partial^{|j_1|+|j_2|} f(x,y)}{\partial x^{j_{11}} \cdots \partial x^{j_{1d_1}} \partial y^{j_{21}} \cdots \partial y^{j_{2d_2}}}$. Throughout, C, c, C_0, c_0, C_1, c_1, L, L_0, L_1, $\ldots$ are generically used to denote positive constants whose values might change from one line to another, but are independent from everything else.

A Simulation

To empirically demonstrate the adaptiveness of the conditional diffusion model to manifold structures, we conduct a simulation study. We first generate a dataset of (x, ϕ), where x is generated from a uniform distribution over $[0, 1]$ and ϕ is generated from a uniform distribution over $[0, 2\pi]$. Given x and ϕ, the response Y is generated by the process

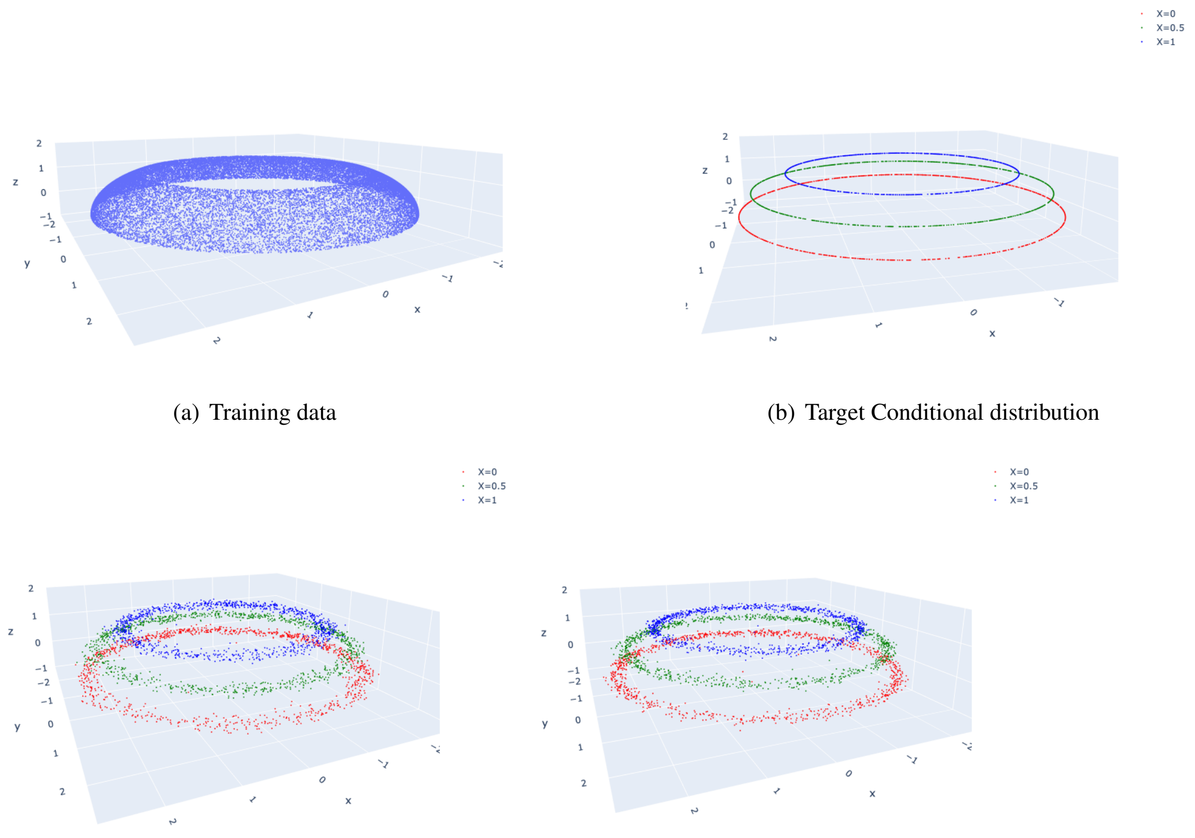
$$Y = ((R + r\cos(x))\cos(\phi), (R + r\sin(x))\sin(\phi), r\sin(x)),$$

where $R = 1$, $r = 1.5$. Then we aim at estimating $Y|x$ and $Y|\phi$. In both examples, we have $D_X = 1$, $D_Y = 3$, and $d_Y = 1$. In particular, given x, the response Y is supported on an ellipse whose radius depends on x. When given ϕ, the response Y is supported on a section of a "tilted" ellipse depending on ϕ.

We then generate $n = 30000$ i.i.d. data points and fit the conditional diffusion model to both examples. We consider two types of conditional score families $\mathcal{S}_{NN}$. The first approach directly models the conditional score function using a ReLU neural network with two hidden layers, where the hidden layer widths are $(128, 64)$. We refer to this approach as NN. The second approach models the conditional score family using a piecewise ReLU neural network, based on our theoretical results. Specifically, we consider

$$\mathcal{S}_{NN} = \left\{ S(y, x, t) = \sum_{i=1}^{\mathcal{I}} S_i(y, x, t) \cdot \mathbf{1}\left(t_{i-1} \le t < t_i\right) \right\}, \tag{1}$$

where $\mathcal{I} = 5$, $t_0 = 0.001$, $t_1 = 0.1$, $t_2 = 0.2$, $t_3 = 0.4$, $t_4 = 1$, $t_5 = 2$. For each $i \in [5]$, S_i is a ReLU neural network with two hidden layers, and the size of the hidden layers decreases with i. Specifically, for i range from 1 to 5, the hidden layer widths are given by $(64, 64)$, $(64, 32)$, $(32, 32)$, $(32, 16)$ and $(16, 16)$, respectively. We refer to this approach as Piecewise NN. The two conditional score families considered above have a comparable number of training parameters. The plots of the generated data from the conditional diffusion model given $x = 0$, $x = 0.5$, and $x = 1$ are shown in Figure 1, and the plots of conditional diffusion model given $\phi = 0$, $\phi = 0.5$, $\phi = 1$ are shown in Figure 2. It is evident that for different values of x (and ϕ), the generated response Y concentrates around distinct ellipse (and tilted ellipse). This indicates that the conditional diffusion model effectively captures both the covariate information and the underlying manifold structure. Table 1 presents the MMD (Maximum Mean Discrepancy) distance[1] between the generated data and the true conditional distribution for different values of x (and ϕ), as well as the average across all values of x (and ϕ). Consistent with our theoretical results, introducing the piecewise structure to the neural network results in a smaller MMD distance.



(a) Training data

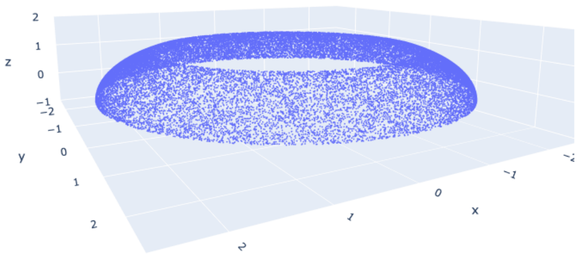
(b) Target Conditional distribution

(c) ReLU NN

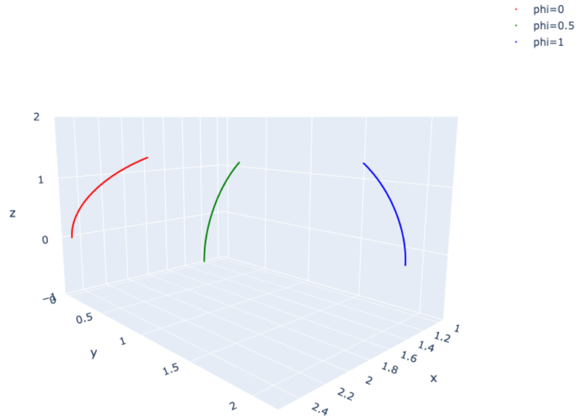
(d) Piecewise ReLU NN

Figure 1: Figure (a) shows the training dataset. Figure (b) displays samples from the (true) conditional distribution $Y \mid x = 0$ (red dots), $Y \mid x = 0.5$ (green dots), and $Y \mid x = 1$ (blue dots). Figure (c) presents samples generated from the conditional diffusion model with the conditional score modeled by a ReLU neural network. Figure (d) illustrates samples generated from the conditional diffusion model with the conditional score modeled by the piecewise ReLU neural network defined in equation (1).

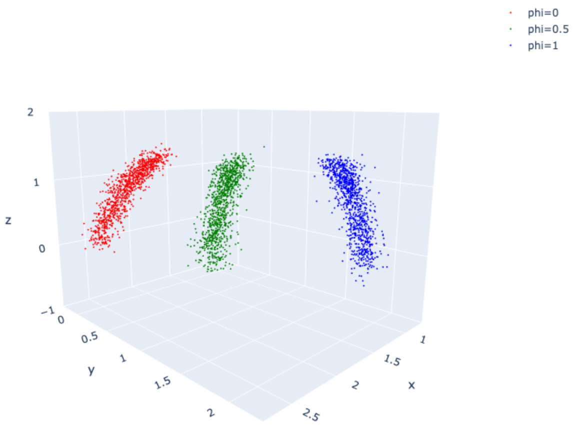
[1]We consider the MMD distance associated with the RBF kernel $\exp(-\|x - y\|^2/6)$.



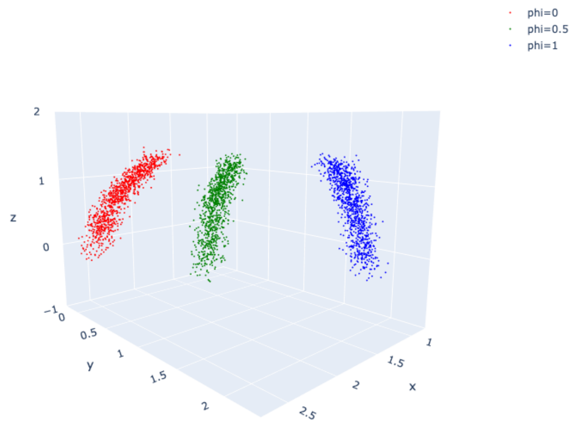
(a) Training data



(b) Target Conditional distribution



(c) ReLU NN



(d) Piecewise ReLU NN

Figure 2: Figure (a) shows the training dataset. Figure (b) displays samples from the (true) conditional distribution $Y \mid \phi = 0$ (red dots), $Y \mid \phi = 0.5$ (green dots), and $Y \mid \phi = 1$ (blue dots). Figure (c) presents samples generated from the conditional diffusion model with the conditional score modeled by a ReLU neural network. Figure (d) illustrates samples generated from the conditional diffusion model with the conditional score modeled by the piecewise ReLU neural network defined in equation (1).

Table 1: The table presents the MMD distances between the conditional diffusion model estimator and the target conditional distribution. The first three rows show the MMD distances for the conditional distributions $Y \mid x = 0$, $Y \mid x = 0.5$, $Y \mid x = 1$ and $Y \mid \phi = 0$, $Y \mid \phi = 0.5$, $Y \mid \phi = 1$. The last row displays the expected conditional MMD distance, where the expectation is taken with respect to x sampled from a uniform distribution on $[0, 1]$ and ϕ sampled from uniform over $[0, 2\pi]$.

	Piecewise NN	NN		Piecewise NN	NN
$x = 0$	0.0023	0.0032	$\phi = 0$	0.0002	0.0034
$x = 0.5$	0.0013	0.0014	$\phi = 0.5$	0.0009	0.0013
$x = 1$	0.0007	0.0017	$\phi = 1$	0.0014	0.0028
$x \sim Unif[0, 1]$	0.0021	0.0031	$\phi \sim Unif[0, 2\pi]$	0.0008	0.0015

B Missing Definition and Assumption

We begin by defining a class of smooth multivariate functions.

Definition 1. *The class $C_L^{\alpha_1,\alpha_2}(U_1,U_2)$ consists of functions $f : U_1 \times U_2 \to \mathbb{R}$ with $U_1 \subset \mathbb{R}^{d_1}$, $U_2 \subset \mathbb{R}^{d_2}$ so that for any $(x_0,y_0) \in U_1 \times U_2$, and each index $(j_1,j_2) \in \mathcal{J}_{\alpha_1,\alpha_2}^{d_1,d_2} = \{j_1 \in \mathbb{N}_0^{d_1}, j_2 \in \mathbb{N}_0^{d_2} : |j_1| + \frac{\alpha_1}{\alpha_2}|j_2| < \alpha_1\}$, there is a number $f_{(j_1,j_2)}(x_0,y_0) \in [-L,L]$ so that for any $(x,y) \in U_1 \times U_2$,*

$$\Big|f(x,y) - \sum_{(j_1,j_2)\in\mathcal{J}_{\alpha_1,\alpha_2}^{d_1,d_2}} \frac{f_{(j_1,j_2)}(x_0,y_0)}{j_1!j_2!}(x-x_0)^{j_1}(y-y_0)^{j_1}\Big| \le L(\|x-x_0\|^{\alpha_1} + \|y-y_0\|^{\alpha_2}).$$

For $d > 1$, we use $C_{L,d}^{\alpha_1,\alpha_2}(U_1,U_2) = \{f = (f_1,f_2,\cdots,f_d) : U_1 \times U_2 \to \mathbb{R}^d : \forall i \in [d], f_i \in C_L^{\alpha_1,\alpha_2}(U_1,U_2)\}$ to denote the vector-valued function space counterpart. We call a (vector-valued) function $f = (f_1,f_2,\cdots,f_d) : U_1 \times U_2 \to \mathbb{R}^d$ being C^{α_1,α_2}-smooth if there exists a constant L so that $f \in C_{L,d}^{\alpha_1,\alpha_2}(U_1,U_2)$.

If $\alpha_X \le 1$, then a conditional density function $p(y|x)$ is C^{α_Y,α_X}-smooth if, for any given x, $p(y|x)$ is α_Y-Hölder smooth with respect to the variable y, and for any y and pair x, x', $|p(y|x) - p(y|x')| \le L\|x - x'\|^{\alpha_X}$. This corresponds to the conditional density class considered in [1]. When $\alpha_X > 1$, the C^{α_Y,α_X} smoothness of a function can be verified by checking the existence and smoothness of its partial derivatives, as summarized in the following lemma.

Lemma B.1. *For a function $f : U_1 \times U_2 \to \mathbb{R}$, if there exists a function $\overline{f} : \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \to \mathbb{R}$ so that $\overline{f}|_{U_1\times U_2} = f$ and*

$$\sum_{(j_1,j_2)\in\mathcal{J}_{\alpha_1,\alpha_2}^{d_1,d_2}} \sup_{(x,y)\in\mathbb{R}^{d_1}\times\mathbb{R}^{d_2}} |\overline{f}^{(j_1,j_2)}(x,y)| + \sum_{\substack{(j_1,j_2)\in\mathcal{J}_{\alpha_1,\alpha_2}^{d_1,d_2} \\ \frac{|j_1|+1}{\alpha_1}+\frac{|j_2|}{\alpha_2}\ge 1}} \sup_{\substack{x,x_0\in\mathbb{R}^{d_1},y\in\mathbb{R}^{d_2} \\ x\neq x_0}} \frac{|\overline{f}^{(j_1,j_2)}(x,y) - \overline{f}^{(j_1,j_2)}(x_0,y)|}{\|x-x_0\|^{\alpha_1-|j_1|-\frac{\alpha_1}{\alpha_2}|j_2|}}$$
$$+ \sum_{\substack{(j_1,j_2)\in\mathcal{J}_{\alpha_1,\alpha_2}^{d_1,d_2} \\ \frac{|j_1|}{\alpha_1}+\frac{|j_2|+1}{\alpha_2}\ge 1}} \sup_{\substack{x\in\mathbb{R}^{d_1},y,y_0\in\mathbb{R}^{d_2} \\ y\neq y_0}} \frac{|\overline{f}^{(j_1,j_2)}(x,y) - \overline{f}^{(j_1,j_2)}(x,y_0)|}{\|y-y_0\|^{\alpha_2-|j_2|-\frac{\alpha_2}{\alpha_1}|j_1|}} \le L,$$

then there exists a constant L_1 so that $f \in C_{L_1}^{\alpha_1,\alpha_2}(U_1,U_2)$.

Proof. For any $(x,y),(x_0,y_0) \in U_1 \times U_2$, we have

$$\Big|\overline{f}(x,y) - \sum_{\substack{j_2\in\mathbb{N}_0^{d_2} \\ |j_2|<\alpha_2}} \frac{\overline{f}^{(0,j_2)}(x,y_0)}{j_2!}(y-y_0)^{j_2}\Big|$$
$$= \Big| \sum_{\substack{j_2\in\mathbb{N}_0^{d_2} \\ |j_2|=\lfloor\alpha_2\rfloor}} \frac{\lfloor\alpha_2\rfloor}{j_2!}\int_0^1 (1-t)^{\lfloor\alpha_2\rfloor-1}\big(\overline{f}^{(0,j_2)}(x,y_0+t(y-y_0)) - \overline{f}^{(0,j_2)}(x,y_0)\big)\,\mathrm{d}t \cdot (y-y_0)^{j_2}\Big|$$
$$= \mathcal{O}(\|y-y_0\|^{\alpha_2}).$$

Moreover, we have

$$\Big| \sum_{\substack{j_2\in\mathbb{N}_0^{d_2}\\ |j_2|<\alpha_2}} \frac{\overline{f}^{(0,j_2)}(x,y_0)}{j_2!}(y-y_0)^{j_2} - \sum_{\substack{j_2\in\mathbb{N}_0^{d_2}\\ |j_2|<\alpha_2}} \sum_{\substack{j_1\in\mathbb{N}_0^{d_1}\\ |j_1|+\frac{\alpha_1}{\alpha_2}|j_2|<\alpha_1}} \frac{\overline{f}^{(j_1,j_2)}(x_0,y_0)}{j_2!}(x-x_0)^{j_1}(y-y_0)^{j_2}\Big|$$

$$= \Big| \sum_{\substack{j_2\in\mathbb{N}_0^{d_2}\\ |j_2|<\alpha_2}} \sum_{\substack{j_1\in\mathbb{N}_0^{d_1}\\ |j_1|=\lfloor\alpha_1-\frac{\alpha_1}{\alpha_2}|j_2|\rfloor}} \frac{\lfloor\alpha_1-\frac{\alpha_1}{\alpha_2}|j_2|\rfloor}{j_1!j_2!}\int_0^1 (1-t)^{\lfloor\alpha_1-\frac{\alpha_1}{\alpha_2}|j_2|\rfloor-1}\big(\overline{f}^{(j_1,j_2)}(x_0+t(x-x_0),y_0)-\overline{f}^{(j_1,j_2)}(x_0,y_0)\big)\,\mathrm{d}t$$

$$\cdot (x-x_0)^{j_1}(y-y_0)^{j_2}\Big|$$

$$= \mathcal{O}\Big(\sum_{\substack{j_2\in\mathbb{N}_0^{d_2}\\ |j_2|<\alpha_2}} \sum_{\substack{j_1\in\mathbb{N}_0^{d_1}\\ |j_1|=\lfloor\alpha_1-\frac{\alpha_1}{\alpha_2}|j_2|\rfloor}} \|x-x_0\|^{\alpha_1-\frac{\alpha_1}{\alpha_2}|j_2|}\|y-y_0\|^{|j_2|}\Big) = \mathcal{O}(\|x-x_0\|^{\alpha_1}+\|y-y_0\|^{\alpha_2}),$$

where the last inequality uses the Young's inequality for products. Therefore, by choosing $f_{(j_1,j_2)}(x_0,y_0) = \overline{f}^{(j_1,j_2)}(x_0,y_0)$, we can get

$$\Big|f(x,y) - \sum_{(j_1,j_2)\in\mathcal{J}^{d_1,d_2}_{\alpha_1,\alpha_2}} \frac{f_{(j_1,j_2)}(x_0,y_0)}{j_1!j_2!}(x-x_0)^{j_1}(y-y_0)^{j_1}\Big|$$

$$= \Big\|\overline{f}(x,y) - \sum_{\substack{j_2\in\mathbb{N}_0^{d_2}\\ |j_2|<\alpha_2}} \sum_{\substack{j_1\in\mathbb{N}_0^{d_1}\\ |j_1|+\frac{\alpha_1}{\alpha_2}|j_2|<\alpha_1}} \frac{\overline{f}^{(j_1,j_2)}(x_0,y_0)}{j_2!}(x-x_0)^{j_1}(y-y_0)^{j_2}\Big\| = \mathcal{O}(\|x-x_0\|^{\alpha_1}+\|y-y_0\|^{\alpha_2}).$$

□

Note that when $\alpha_1 = \alpha_2 = \alpha$, the function class considered in Lemma B.1 is the conventional Hölder class with Hölder exponent being α. Then we present the formal version of Assumption D for the analysis of the conditional diffusion model under the manifold assumption.

Assumption D (Smoothness of $\mu^*_{Y|X}$): For any $x \in \mathcal{M}_X$, $\mathcal{M}_{Y|x}$ is a compact boundaryless d_Y-dimensional submanifold embedded in $\mathbb{R}^{D_Y}$ with reach bounded away from zero. Moreover, there exists positive constants $(c_1, c_2, r_0, r_1, L, L_1, L_2, L_3)$ so that for any $w = (x_0, y_0) \in \mathcal{M}$, there exists a open set U^ω on $\mathcal{M}$ so that

1. $\mathbb{B}_{\mathcal{M}_X}(x_0, r_0) \subset U^\omega_X$ and for any $x \in U^\omega_X$, $\mathbb{B}_{\mathcal{M}_{Y|x}}(y_0, r_0) \subset U^\omega_{Y|x}$.
2. For any $x \in U^\omega_X$, there exists a uniformly L-Lipschitz diffeomorphism Q^ω_x that maps $U^\omega_{Y|x}$ to $\mathbb{B}_{\mathbb{R}^{d_Y}}(0, r_1)$ with inverse $[Q^\omega_x]^{-1}$ so that $Q^\omega_{x_0}(y_0) = 0$ and
   (a) The function $G^\omega : \mathbb{B}_{\mathbb{R}^{d_Y}}(0, r_1) \times U^\omega_X \to U^\omega_Y$ defined as $G^\omega(z, x) = [Q^\omega_x]^{-1}(z)$ satisfies that $G^\omega \in C^{\beta_Y,\beta_X}_{L_1,D_Y}(\mathbb{B}_{\mathbb{R}^{d_Y}}(0, r_1), U^\omega_X)$.
   (b) For any $x \in \mathcal{M}_X$, $\mu^*_{Y|x}$ have a density $f(y|x)$ with respect to the volume measure of $\mathcal{M}_{Y|x}$ so that $f(y|x)$ is uniformly lower bounded by c_1. Moreover, the function v^ω : $\mathbb{B}_{\mathbb{R}^{d_Y}}(0, r_1) \times U^\omega_X \to \mathbb{R}$ defined by $v^\omega(z, x) = f([Q^\omega_x]^{-1}(z)|x) \cdot \sqrt{\det(J_x(z)^T J_x(z))}$ with $J_x(z) = J_{[Q^\omega_x]^{-1}}(z)$ being the Jacobian matrix of $[Q^\omega_x]^{-1}(\cdot)$ evaluated at z, satisfies that $v^\omega \in C^{\alpha_Y,\alpha_X}_{L_2}(\mathbb{B}_{\mathbb{R}^{d_Y}}(0, r_1), U^\omega_X)$.

Remark B.1. *Intuitively, this assumption implies that, locally around any point $\omega = (x_0, y_0) \in \mathcal{M}$, there exists an encoder-dencoder pair $(G^\omega(z, x), Q^\omega_x(y))$. Here, $Q^\omega_x(\cdot)$ maps $y \in \mathbb{B}_{\mathcal{M}_{Y|x}}(y_0, r_0)$ to a low dimensional code $z \in \mathbb{R}^{d_Y}$, and $G^\omega(\cdot, x)$ reconstruct the data y from the code z. A large β_Y implies* *that, for any given $x \in \mathcal{M}_X$, the manifold $M_{Y|x}$ is smooth. On the other hand, a large β_X indicates that the space $M_{Y|x}$ changes smoothly with x, meaning $\mathcal{M}_{Y|x}$ and $\mathcal{M}_{Y|x'}$ will be similar if x is close to x' in Euclidean distance. Moreover, $v^\omega(z|x) = v^\omega(z, x)$ is the conditional density function of the (local) latent vector, that is, the density of the push forward measure $[Q_x^\omega]_\#(\mu^*_{Y|x}|_{U^\omega_{Y|x}})$ with respect to the Lebesgue measure on $\mathbb{R}^{d_Y}$, where $\mu^*_{Y|x}|_{U^\omega_{Y|x}}$ is the measure of $\mu^*_{Y|x}$ constrained on $U^\omega_{Y|x}$, defined by $\frac{\mathrm{d}\mu^*_{Y|x}|_{U^\omega_{Y|x}}}{\mathrm{d}\mu^*_{Y|x}} = \mathbf{1}(y \in U^\omega_{Y|x})$. Therefore, a large α_Y indicates that the conditional density function will be smooth for any fixed x, while a large α_X means that the density function changes smoothly in x. Under Assumption D, we can express $\mu^*_{Y|X}$ as a mixture of (deterministic) conditional generative model, as shown in the following lemma.*

Lemma B.2. *(Expressing $\mu^*_{Y|X}$ as conditional generative model) For any r with $0 < r \le r_0$, it holds that*

1. *For any $(x^*, y^*) \in \mathcal{M}$ and $x \in \mathbb{B}_{\mathcal{M}_X}(x^*, r_0)$, it holds for any measurable function $g : \mathcal{M}_{Y|x} \to \mathbb{R}$ that*

$$\mathbb{E}_{y\sim\mu^*_{Y|x}}[g(y)\cdot\mathbf{1}(y \in \mathbb{B}_{\mathcal{M}_{Y|x}}(y^*, r))] = \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} g(G^*(z, x))\mathbf{1}(G^*(z, x) \in \mathbb{B}_{\mathcal{M}_{Y|x}}(y^*, r)))v^*(z|x)\,\mathrm{d}z,$$

   where $G^* = G^\omega$ and $v^* = v^\omega$ with $\omega = (x^*, y^*)$.

2. *For any function $\rho : \mathbb{R} \to [0, 1]$ satisfies when $t \in [0, 1]$, $\rho(t) = 1$ and when $t \in [2, \infty)$, $\rho(t) = 0$. Let $\{(x^*_k, y^*_k)\}_{k=1}^K \subset \mathcal{M}$ be a $\frac{r}{2}$-cover of $\mathcal{M}$. Then for any $\widetilde{r}$ satisfies $r \le \widetilde{r} \le r_0$, denote*

$$\rho_k(x, y) = \rho(\frac{4\|x - x^*_k\|^2}{\widetilde{r}^2})\rho(\frac{4\|y - y^*_k\|^2}{\widetilde{r}^2})$$

   and $\widetilde{\rho}_k = \rho_k / \sum_{k=1}^K \rho_k$, it holds for any measurable function $g : \mathcal{M}_{Y|x} \to \mathbb{R}$ that

$$\mathbb{E}_{y\sim\mu^*_{Y|x}}[g(y)] = \sum_{k=1}^K \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} g(G^*_{[k]}(z, x))\widetilde{\rho}_k(x, G^*_{[k]}(z, x))v^*_{[k]}(z|x)\,\mathrm{d}z,$$

   where $G^*_{[k]} = G^\omega$ and $v^*_{[k]} = v^\omega$ with $\omega = (x^*_k, y^*_k)$.

C Proof of Theorem 2

Denote μ^*_X as the distribution of X, and $\mu^* = \mu^*_X\mu^*_{Y|X}$ as the joint distribution of (X, Y). We only need to consider the case where $\beta_Y = \alpha_Y \vee 1 + 1$ and $\beta_X = \alpha_X + \frac{\alpha_X}{\alpha_Y}$. Set

$$\tau = (n^{-\frac{1}{2\alpha_Y + d_Y + \frac{\alpha_Y}{\alpha_X} d_X}} \sqrt{\log n})^{2(\alpha_Y+1)}.$$

We have the following lemma that relate the generalization error of the conditional score function $\nabla \log p_{t|x}(w)$ to the generalization error of $\mu^*_{Y|x}$.

Lemma C.1. *Suppose for any $t \in [\tau, T]$, $\sup_{w\in\mathbb{R}^{D_Y}} \sup_{x\in\mathcal{M}_X} \|\widehat{S}(w, x, t)\| \lesssim \sqrt{\frac{\log n}{t\wedge 1}}$, then let $\mu^\tau_{Y|x}$ be the distribution of $\overleftarrow{Y}_{\tau|x}$, we have*

$$\mathbb{E}_{\mu^*_X}[\mathrm{TV}\left(\widehat{\mu}_{Y|x}, \mu^*_{Y|x}\right)] \lesssim \frac{1}{n} + \mathbb{E}_{\mu^*_X}[\mathrm{TV}(\mu^*_{Y|x}, \mu^\tau_{Y|x})]$$
$$+ \mathbb{E}_{\mu^*_X}\left[\sum_{i=0}^{K-1} \sqrt{\int_{t_i}^{t_{i+1}} \int_{\mathbb{R}^{D_Y}} \left\|\widehat{S}(w, x, t) - \nabla \log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\,\mathrm{d}t}\right].$$

and

$$\mathbb{E}_{\mu_X^*}[W_1\left(\widehat{\mu}_{Y|x},\mu^*_{Y|x}\right)]\lesssim\frac{1}{n}+\tau^{\frac{1}{2}}$$
$$+\,\mathbb{E}_{\mu_X^*}\left[\sum_{i=0}^{K-1}\sqrt{\left((t_i\log n)\wedge 1\right)\int_{t_i}^{t_{i+1}}\int_{\mathbb{R}^{D_Y}}\left\|\widehat{S}(w,x,t)-\nabla\log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\,\mathrm{d}t}\right].$$

The proof of Lemma C.1 directly follows from Lemma D.7 of [2] and Lemma B.2 of [4]. Then the following lemma provides upper bounds to the score approximation error.

Lemma C.2. *For any $t\in[\underline{t},\bar{t}]$ with $1<\frac{\bar{t}}{\underline{t}}\le 2$:*

1. *If $\tau\le\underline{t}<n^{-\frac{2}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}}$, there exists a neural network $\phi_{score}(w,x,t)\in\Phi(H,W,R,B,V)$ satisfying*
$$\mathbb{E}_{\mu_X^*}\left[\int_{\underline{t}}^{\bar{t}}\int_{\mathbb{R}^{D_Y}}\left\|\phi_{score}(w,x,t)-\nabla\log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\mathrm{d}t\right]$$
$$=\widetilde{\mathcal{O}}\Big(\frac{\varepsilon_2^{2\beta_X}+\varepsilon_1^{2\beta_Y}}{\underline{t}}+\varepsilon_1^{2\alpha_Y}\Big),$$
where $\varepsilon_1=n^{-\frac{1}{2\alpha_Y+d_Y+\frac{\alpha_Y}{\alpha_X}d_X}}$ and $\varepsilon_2=\varepsilon_1^{\frac{\alpha_Y}{\alpha_X}}$. Here H, W, R, B and V are evaluated as $H=\Theta\left(\log^4 n\right)$, $\|W\|_\infty=\widetilde{\Theta}\big(\varepsilon_1^{-d_Y}\varepsilon_2^{-d_X}\big)$, $R=\widetilde{\Theta}\big(\varepsilon_1^{-d_Y}\varepsilon_2^{-d_X}\big)$, $B=\exp\left(\Theta(\log^4 n)\right)$ and $V=\Theta(\sqrt{\frac{\log n}{\underline{t}}})$.

2. *If $n^{-\frac{2}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}}\le\underline{t}\le(\log n)^{-3}$, there exists a neural network $\phi_{score}(w,x,t)\in\Phi(H,W,R,B,V)$ satisfying*
$$\mathbb{E}_{\mu_X^*}\left[\int_{\underline{t}}^{\bar{t}}\int_{\mathbb{R}^{D_Y}}\left\|\phi_{score}(w,x,t)-\nabla\log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\mathrm{d}t\right]=\widetilde{\mathcal{O}}(\varepsilon_2^{2\alpha_X}),$$
with $\varepsilon_2=\widetilde{\Theta}(n^{-\frac{1}{2\alpha_X+d_X}}\underline{t}^{-\frac{d_Y}{4\alpha_X+2d_X}})$. Here H, W, R, B and V are evaluated as $H=\Theta\left(\log^4 n\right)$, $\|W\|_\infty=\widetilde{\Theta}\big(\underline{t}^{-\frac{d_Y}{2}}\varepsilon_2^{-d_X}\big)$, $R=\widetilde{\Theta}\big(\underline{t}^{-\frac{d_Y}{2}}\varepsilon_2^{-d_X}\big)$, $B=\exp\left(\Theta(\log^4 n)\right)$ and $V=\Theta(\sqrt{\frac{\log n}{\underline{t}}})$.

3. *If $(\log n)^{-3}\le\underline{t}\le T=\Theta(\log n)$, there exists a neural network $\phi_{score}(w,x,t)\in\Phi(H,W,R,B,V)$ satisfying*
$$\mathbb{E}_{\mu_X^*}\left[\int_{\underline{t}}^{\bar{t}}\int_{\mathbb{R}^{D_Y}}\left\|\phi_{score}(w,x,t)-\nabla\log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\mathrm{d}t\right]=\widetilde{\mathcal{O}}(n^{-\frac{2\alpha_X}{2\alpha_X+d_X}}).$$
Here H, W, R, B and V are evaluated as $H=\Theta\big(\log^4 n\big)$, $\|W\|_\infty=\widetilde{\Theta}\big(n^{\frac{d_X}{2\alpha_X+d_X}}\big)$, $R=\widetilde{\Theta}\big(n^{\frac{d_X}{2\alpha_X+d_X}}\big)$, $B=\exp\left(\Theta(\log^4 n)\right)$ and $V=\Theta(\sqrt{\frac{\log n}{\underline{t}\wedge 1}})$.

Then denote $\mathcal{S}_i=\Phi(H_i,W_i,R_i,B_i,V_i)$, by Lemma C.2, we have for any $i\in[\mathcal{I}]$,

$$\left((t_i\log n)\wedge 1\right)\cdot\min_{S\in\mathcal{S}_i}\mathbb{E}_{\mu_X^*}\left[\int_{t_{i-1}}^{t_i}\int_{\mathbb{R}^{D_Y}}\|S(w,x,t)-\nabla\log p_{t|x}(w)\|^2 p_{t|x}(w)\,\mathrm{d}t\mathrm{d}w\right]$$
$$=\begin{cases}\widetilde{\mathcal{O}}\Big(n^{-\frac{2+\frac{2}{\alpha_Y}}{2+\frac{d_X}{\alpha_X}+\frac{d_Y}{\alpha_Y}}}\Big), & \tau\le t_{i-1}<n^{-\frac{2}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}};\\ \widetilde{\mathcal{O}}\Big(n^{-\frac{2\alpha_X}{2\alpha_X+d_X}}+n^{-\frac{2+\frac{2}{\alpha_Y}}{2+\frac{d_X}{\alpha_X}+\frac{d_Y}{\alpha_Y}}}\Big) & n^{-\frac{2}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}}\le t_{i-1}<\frac{c}{\log n}\\ \widetilde{\mathcal{O}}\Big(n^{-\frac{2\alpha_X}{2\alpha_X+d_X}}\Big) & \frac{c}{\log n}\le t_{i-1}\le T\end{cases}$$

Then we derive the following oracle inequality for bounding the estimation error.

Lemma C.3. *It holds with probability larger than $1 - \frac{1}{n}$ that for any $i \in [\mathcal{I}]$,*

$$
\begin{aligned}
&\mathbb{E}_{\mu_X^*}\Big[\int_{t_{i-1}}^{t_i}\int_{\mathbb{R}^{D_Y}} \|\widehat{S}(w,x,t) - \nabla \log p_{t|x}(w)\|^2\, p_{t|x}(w)\,\mathrm{d}t\mathrm{d}w\Big] \\
&\lesssim (\log n)^2 \frac{R_i H_i \log\left(R_i H_i \|W_i\|_\infty (B_i \vee 1) n\right)}{n} \\
&\qquad + \min_{S\in\mathcal{S}_i} \mathbb{E}_{\mu_X^*}\Big[\int_{t_{i-1}}^{t_i}\int_{\mathbb{R}^{D_Y}} \|S(w,x,t) - \nabla \log p_{t|x}(w)\|^2\, p_{t|x}(w)\,\mathrm{d}t\mathrm{d}w\Big]
\end{aligned}
$$

So by combining all pieces, we have

$$
\begin{aligned}
\mathbb{E}_{\mu_X^*}[W_1(\widehat{\mu}_{Y|x}, \mu_{Y|x}^*)] &\lesssim \tau^{\frac{1}{2}} + \frac{1}{n} \\
&\quad + \mathbb{E}_{\mu_X^*} \sum_{i=1}^{\mathcal{I}} \sqrt{\left((t_i \log n) \wedge 1\right) \int_{t_{i-1}}^{t_i}\int_{\mathbb{R}^{D_Y}} \left\|\widehat{S}(w,x,t) - \nabla \log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\,\mathrm{d}t} \\
&\lesssim \tau^{\frac{1}{2}} + \sum_{i=1}^{\mathcal{I}} (\log n) \sqrt{\left((t_i \log n) \wedge 1\right) \frac{R_i H_i \log\left(R_i H_i \|W_i\|_\infty (B_i \vee 1) n\right)}{n}} \\
&\quad + \sum_{i=1}^{\mathcal{I}} \sqrt{\left((t_i \log n) \wedge 1\right) \min_{S\in\mathcal{S}_i} \mathbb{E}_{\mu_X^*}\Big[\int_{t_{i-1}}^{t_i}\int_{\mathbb{R}^{D_Y}} \|S(w,x,t) - \nabla \log p_{t|x}(w)\|^2\, p_{t|x}(w)\,\mathrm{d}t\mathrm{d}w\Big]} \\
&= \widetilde{\mathcal{O}}\Big(n^{-\frac{\alpha_X}{2\alpha_X + d_X}} + n^{-\frac{\alpha_Y + 1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}}\Big).
\end{aligned}
$$

C.1 Proof of Lemma C.2

To begin with, we introduce the following lemma, which states that it is sufficient to approximate the score function $\nabla \log p_{t|x}(w)$ only for values of w that are in close proximity to the manifold $\mathcal{M}_{Y|x}$.

Lemma C.4. *If* $\sup_{w\in\mathbb{R}^{D_Y}, x\in\mathcal{M}_X} \sup_{t\in[\tau,T]} [\|S(w,x,t)\|_\infty \sigma_t] \le c\sqrt{\log n}$. *Then, there exist constants* (c_0, c_1, c_2, c_3) *so that for any $i \in [\mathcal{I}]$ and $t \in [t_{i-1}, t_i]$ with $1 < \frac{t_i}{t_{i-1}} \le 2$,*

1. *Denote* $\mathrm{dist}(w, \mathcal{M}_{Y|x})$ *as the distance of point $w \in \mathbb{R}^{D_Y}$ to manifold $\mathcal{M}_{Y|x}$. Then for any $x \in \mathcal{M}_X$,*

$$
\begin{aligned}
&\int_{\mathbb{R}^{D_Y}} \left\|\nabla \log p_{t|x}(w) - S(w,x,t)\right\|^2 p_{t|x}(w)\,\mathrm{d}w \\
\le &\int_{\mathbb{R}^{D_Y}} \left\|\nabla \log p_{t|x}(w) - S(w,x,t)\right\|^2 p_{t|x}(w) \cdot 1\left(\mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0 \sigma_{t_{i-1}} \sqrt{\log n}\right) \mathrm{d}w \\
&\qquad + (1 + c^2) \cdot c_1 \frac{1}{n^2}.
\end{aligned}
$$

2. *For any $x \in \mathcal{M}_X$ and $w \in \mathbb{R}^{D_Y}$ satisfying* $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0 \sigma_{t_{i-1}} \sqrt{\log n}$, *we have*

   (a) $\|\nabla \log p_{t|x}(w)\|_\infty \le c_2 \frac{\sqrt{\log n}}{\sigma_{t_{i-1}}}$.

   (b) $(2\pi\sigma_t^2)^{\frac{D}{2}} p_{t|x}(w) \ge n^{-c_3}$.

Then the following lemma gives a way for constructing covering set to $\mathcal{M}_{Y|X}$.

Lemma C.5. *Under Assumptions C and D, there exist positive constants $r, \overline{r}, L_1$ satisfying $r \le \frac{r_0}{4}$ and $\overline{r} \le \frac{r_1}{2}$, so that for any $\varepsilon_1 \in (0, \overline{r})$, $\varepsilon_2 \in (0, r)$, let $\mathcal{N}_{\varepsilon_1}^Z$ be an ε_1-cover of $\mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$, $\mathcal{N}_{\varepsilon_2}^X$ be an ε_2-cover of $\mathcal{M}_X$ and $\{(x_k^*, y_k^*)\}_{k=1}^K \subset \mathcal{M}$ be any r-cover of $\mathcal{M}$, we have*

1. *for any* $k \in [K]$ *and* $x \in U_X^{(x_k^*, y_k^*)}$, $z \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, r_1)$,

$$\lambda_{\min}\big(J_{G^{(x_k^*,y_k^*)}(\cdot,x)}(z)^T J_{G^{(x_k^*,y_k^*)}(\cdot,x)}(z)\big) \geq \frac{1}{L^2}.$$

2. *for any* $k \in [K]$ *and* $(x, y) \in \mathcal{M}$ *so that* $\|x - x_k^*\| \leq r$ *and* $\|y - y_k^*\| \leq r$, *it holds that* $Q_x^{(x_k^*,y_k^*)}(y) \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$.

3. *for any* $(x, y) \in \mathcal{M}$, *there exists* $x^* \in \mathcal{N}_{\varepsilon_2}^X$, $k \in \mathcal{K}_{x^*} = \{k \in [K] : \|x^* - x_k^*\| \leq 2r\}$ *and* $z^* \in \mathcal{N}_{\varepsilon_1}^Z$ *so that* $\|x - x^*\| \leq \varepsilon_2$ *and* $\|G^{(x_k^*,y_k^*)}(z^*, x) - y\| \leq L_1\varepsilon_1$.

4. *for any* $x^* \in \mathcal{N}_{\varepsilon_2}^X$ *and* $k \in \mathcal{K}_{x^*}$, *if* $x \in \mathcal{B}_{\mathcal{M}_X}(x^*, \varepsilon_2)$ *and* $z \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$, *then* $\|G^{(x_k^*,y_k^*)}(z, x) - y_k^*\| \leq \frac{r_0}{2}$.

In the following analysis, we will fix an r-cover $\{(x_k^*, y_k^*)\}_{k=1}^K \subset \mathcal{M}$ of $\mathcal{M}$: and let $\mathcal{K}_{x^*} = \{k \in [K] : \|x^* - x_k^*\| \leq 2r\}$, where r is the positive constant required in Lemma C.5. For each $k \in [K]$, we denote $U_{[k]}^* = U^{(x_k^*,y_k^*)}$,

$$G_{[k]}^*(z, x) = G^{(x_k^*,y_k^*)}(z, x), \qquad Q_{[k]}^*(y, x) = Q_x^{(x_k^*,y_k^*)}(y),$$

and

$$v_{[k]}^*(z|x) = v^{(x_k^*,y_k^*)}(z|x),$$

where $U^{(x_k^*,y_k^*)}$, $G^{(x_k^*,y_k^*)}(z, y)$, $Q_x^{(x_k^*,y_k^*)}(y)$ and $v^{(x_k^*,y_k^*)}(z|x)$ are defined in Assumption D with $\omega = (x_k^*, y_k^*)$. Then let us fix a time interval $t \in [\underline{t}, \overline{t}]$ where $1 < \frac{\overline{t}}{\underline{t}} \leq 2$. According to Lemma C.4, it suffices to focus on approximating the score function for $t \in [\underline{t}, \overline{t}]$, $x \in \mathcal{M}_X$ and $w \in \mathbb{R}^{D_Y}$ with $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \leq c_0\sigma_{\underline{t}}\sqrt{\log n}$. Our first objective is to demonstrate that if there are neural networks capable of accurately approximating $\nabla \log p_{t|x}(w)$ for (x, w) lies within local neighborhoods in $\mathcal{M}$, then there exists a neural network capable of providing a reliable approximation of $\nabla \log p_{t|x}(w)$ for all (x, w) satisfying $x \in \mathcal{M}_X$ and $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \leq c_0\sigma_{\underline{t}}\sqrt{\log n}$, this is summarized in the following lemma.

Lemma C.6. *Suppose* $\tau \leq \underline{t} \leq T$, $\varepsilon_2 \in (0, r)$, *and* $\varepsilon_1 \geq \sigma_{\underline{t}}\sqrt{\log n} + \varepsilon_2^{\beta_X}$. *Let* $\mathcal{N}_{\varepsilon_2}^X = (\widetilde{x}_1, \widetilde{x}_2, \cdots, \widetilde{x}_{J_2})$ *be one of the largest* ε_2*-packing of* $\mathcal{M}_X$, *and let* $\mathcal{N}_{\varepsilon_1}^Z = (\widetilde{z}_1, \widetilde{z}_2, \cdots, \widetilde{z}_{J_1})$ *be one of the largest* ε_1*-packing of* $\mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$. *Then if for any* $j_1 \in [J_1]$ *and* $j_2 \in [J_2]$, $k \in \mathcal{K}_{\widetilde{x}_{j_2}}$, *there exists a neural network* $\phi_{kj_1j_2}^*(w, x, t) \in \Phi\big(H, W, R, B, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ *so that for any* $t \in [\underline{t}, \overline{t}]$, $x \in \mathbb{B}_{\mathcal{M}_X}(\widetilde{x}_{j_2}, \sqrt{2}\varepsilon_2)$ *and* $w \in \mathbb{R}^{D_Y}$ *with* $\|w - G_{[k]}^*(\widetilde{z}_{j_1}, x)\| \leq \sqrt{2}(2\varepsilon_1 L_1 + c_0\sigma_{\underline{t}}\sqrt{\log n})$ *and* $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \leq c_0\sigma_{\underline{t}}\sqrt{\log n}$, *it holds that*

$$\|\phi_{kj_1j_2}^*(w, x, t) - \nabla \log p_{t|x}(w)\|_\infty \leq \varepsilon.$$

Then there exists a neural network $\phi_{\mathrm{score}}(w, x, t) \in \Phi\big(H_1, W_1, R_1, B_1, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ *with* $H_1 = \Theta(H + \log^2 n)$, $\|W_1\|_\infty = \Theta(J_1J_2(\|W\|_\infty + \log n) + \log^3 n)$, $R_1 = \Theta(J_1J_2(R + \log n) + \log^4 n)$ *and* $B_1 = \exp(\Theta(\log^2 n)) \vee B$, *so that for any* $t \in [\underline{t}, \overline{t}]$, $x \in \mathcal{M}_X$ *and* $w \in \mathbb{R}^{D_Y}$ *satisfying* $\mathrm{dist}(x, \mathcal{M}_{Y|x}) \leq c_0\sigma_{\underline{t}}\sqrt{\log n}$, *it holds that*

$$\|\phi_{\mathrm{score}}(w, x, t) - \nabla \log p_{t|x}(w)\|_\infty \lesssim \varepsilon + \frac{1}{n}.$$

Now recall that

$$\nabla \log p_{t|x}(w) = \frac{\nabla p_{t|x}(w)}{p_{t|x}(w)},$$

where

$$\nabla p_{t|x}(w) = (2\pi\sigma_t^2)^{-\frac{D}{2}}\mathbb{E}_{y\sim\mu_{Y|x}^*}\left[\exp\left(-\frac{\|w - m_t y\|^2}{2\sigma_t^2}\right) \cdot -\frac{(w - m_t y)}{\sigma_t^2}\right],$$

and

$$p_{t|x}(w) = (2\pi\sigma_t^2)^{-\frac{D}{2}} \mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w - m_t y\|^2}{2\sigma_t^2}\right)\right],$$

with $m_t = \exp\big(-\int_0^t \beta_s \,\mathrm{d}s\big)$ and $\sigma_t^2 = 1 - m_t^2$, which satisfies $1 - m_t \asymp t \wedge 1$ and $\sigma_t \asymp \sqrt{t \wedge 1}$. By statement 2 of Lemma C.4, there exists a large enough constant c_2, so that for any $t \in [\underline{t}, \overline{t}]$, $x \in \mathcal{M}_X$, $w \in \mathbb{R}^{D_Y}$ with $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \leq c_0\sigma_{\underline{t}}\sqrt{\log n}$, and any partition $\{\mathcal{A}_{(x,w)}, \mathcal{M}_{Y|x}\backslash\mathcal{A}_{(x,w)}\}$ of $\mathcal{M}_{Y|x}$ satisfying $\{y \in \mathcal{M}_{Y|x} : \|y - w\| \leq c_2\sigma_{\underline{t}}\sqrt{\log n}\} \subset \mathcal{A}_{w,x}$, it holds that

$$\left\|\nabla \log p_{t|x}(w) - \frac{1}{\sigma_t}\cdot\frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w-m_t y)}{\sigma_t}\mathbf{1}(y\in\mathcal{A}_{(x,w)})\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\mathbf{1}(y\in\mathcal{A}_{(x,w)})\right]}\right\| \leq \frac{1}{n}. \tag{2}$$

We will approximate $\nabla \log p_{t|x}(w)$ by constructing suitable sets $\mathcal{A}_{(x,w)}$ and considering the approximation of $\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w-m_t y)}{\sigma_t}\mathbf{1}(y\in\mathcal{A}_{(x,w)})\right]$ and $\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\mathbf{1}(y\in\mathcal{A}_{(x,w)})\right]$ separately. To achieve this, we will utilize the following lemmas concerning the approximation theorem of neural networks for some standard functions.

Lemma C.7. *(Lemma 3.3 in [2]) There exist neural networks $\phi_m(t), \phi_\sigma(t) \in \Phi(H, W, B, R)$ that approximates m_t and σ_t up to ε for all $t \geq 0$, where $H = \mathcal{O}\left(\log^2\left(\varepsilon^{-1}\right)\right), \|W\|_\infty = \mathcal{O}\left(\log^3\left(\varepsilon^{-1}\right)\right), R = \mathcal{O}\left(\log^4\left(\varepsilon^{-1}\right)\right)$, and $B = \exp\left(\mathcal{O}\left(\log^2\left(\varepsilon^{-1}\right)\right)\right)$.*

Lemma C.8. *(Lemma F.12 in [2]) Take $\varepsilon > 0$ arbitrarily. There exists a neural network $\phi_{\exp} \in \Phi(H, W, R, B)$ such that*

$$\sup_{x,x'\geq 0}\left|e^{-x'} - \phi_{\exp}(x)\right| \leq \varepsilon + |x - x'|$$

holds, where $H = \mathcal{O}\left(\log^2 \varepsilon^{-1}\right), \|W\|_\infty = \mathcal{O}\left(\log \varepsilon^{-1}\right), R = \mathcal{O}\left(\log^2 \varepsilon^{-1}\right), B = \exp\left(\mathcal{O}\left(\log^2 \varepsilon^{-1}\right)\right)$. Moreover, $|\phi_{\exp}(x)| \leq \varepsilon$ for all $x \geq \log 3\varepsilon^{-1}$.

Lemma C.9. *(Lemma F.6 in [2]) Let $d \geq 2, C \geq 1, 0 < \varepsilon_{error} \leq 1$. For any $\varepsilon > 0$, there exists a neural network $\phi_{mult}\left(x_1, x_2, \cdots, x_d\right) \in \Phi(H, W, R, B)$ with $H = \mathcal{O}\left(\log d\left(\log \varepsilon^{-1} + d\log C\right)\right), \|W\|_\infty = 48d$, $R = \mathcal{O}\left(d\log \varepsilon^{-1} + d\log C\right), B = C^d$ such that*

$$\left|\phi_{mult}\left(x_1', x_2', \cdots, x_d'\right) - \prod_{d'=1}^{d} x_{d'}\right| \leq \varepsilon + dC^{d-1}\varepsilon_{error}, \text{ for all } x \in [-C, C]^d \text{ and } x' \in \mathbb{R} \text{ with } \left\|x - x'\right\|_\infty \leq \varepsilon_{error},$$

and $|\phi_{mult}(x)| \leq C^d$ for all $x \in [-C, C]$. Note that some of $x_i, x_j (i \neq j)$ can be shared. For $\prod_{i=1}^{I} x_i^{\omega_i}$ with $\omega_i \in \mathbb{Z}_+ (i = 1, 2, \cdots, I)$ and $\sum_{i=1}^{I}\omega_i = d$, there exists a neural network satisfying the same bounds as above, and the network is denoted by $\phi_{mult}(x;\omega)$.

Lemma C.10. *(Lemma F.7 in [2]) For any $0 < \varepsilon < 1$, there exists $\phi_{rec} \in \Phi(H, W, R, B)$ with $H \leq \mathcal{O}\left(\log^2 \varepsilon^{-1}\right), \|W\|_\infty = \mathcal{O}\left(\log^3 \varepsilon^{-1}\right), R = \mathcal{O}\left(\log^4 \varepsilon^{-1}\right)$, and $B = \mathcal{O}\left(\varepsilon^{-2}\right)$ such that*

$$\left|\phi_{rec}\left(x'\right) - \frac{1}{x}\right| \leq \varepsilon + \frac{|x' - x|}{\varepsilon^2}, \quad \text{for all } x \in \left[\varepsilon, \varepsilon^{-1}\right] \text{ and } x' \in \mathbb{R}.$$

We are then ready to construct neural networks for approximating $\nabla \log p_{t|x}(w)$ for $t \in [\underline{t}, \overline{t}]$, where $\underline{t}$ takes on different values.

C.1.1 Case 1: $c(\log n)^{-1} \le \underline{t} \le T$ with c being a samll enough positive constant

Set $\varepsilon_2 = n^{-\frac{1}{2\alpha_X + d_X}}$ and let $\mathcal{N}_{\varepsilon_2}^X$ be one of the largest ε_2-packing of $\mathcal{M}_X$, we have $J_2 := |\mathcal{N}_{\varepsilon_2}^X| \lesssim \varepsilon_2^{-d_X}$. Then take an arbitrary $\widetilde{x} \in \mathcal{N}_{\varepsilon_2}^X$, we claim that

Claim 1. *For any* $0 \le \delta < \frac{\frac{\alpha_X}{\alpha_Y} \wedge \frac{1}{2}}{2\alpha_X + d_X}$*, let* $\varepsilon_1 = c_1 n^{-\delta}(\log n)^{-1}$, $\mathscr{L}_1 = \frac{\alpha_X \log \varepsilon_2}{\log(\varepsilon_1^2) - \log(\sigma_{\underline{t}}^2)}$, $\mathscr{L}_2 = \frac{\alpha_X \log \varepsilon_2}{\log(\varepsilon_1\sqrt{\log n}) - \log(\sigma_{\underline{t}})}$ *and* $\mathscr{L} = \mathscr{L}_1 \mathscr{L}_2 \cdot (2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\binom{\mathscr{L}_2 + D_Y}{D_Y}\binom{(2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\lfloor \beta_X \rfloor + \lceil 2\beta_X \rceil + \lfloor \alpha_X \rfloor + D_X}{D_X}$*, then when* c_1 *is small enough, there exists a network* $\phi^*(w, x, t) \in \Phi(H, W, R, B, V)$ *with* $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta\big(\log^6 n \mathscr{L} \varepsilon_1^{-d_Y}\big)$, $R = \Theta\big(\log^8 n \mathscr{L} \varepsilon_1^{-d_Y}\big)$, $B = \exp(\Theta(\log^4 n))$ *and* $V = \Theta(\sqrt{\frac{\log n}{\underline{t} \wedge 1}})$*, so that for any* $t \in [\underline{t}, \overline{t}]$ *and* $(x, w) \in \{x \in \mathcal{M}_X, w \in \mathbb{R}^{D_Y} : \|x - \widetilde{x}\| \le \varepsilon_2, \mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0 \sigma_{\underline{t}} \sqrt{\log n}\}$,

$$\|\phi^*(w, x, t) - \nabla \log p_{t|x}(w)\|_\infty = \mathcal{O}(\varepsilon_2^{\alpha_X} \log n).$$

Then by $J_2 = \mathcal{O}\big(\varepsilon_2^{-d_X}\big)$ and Lemma C.6, by setting $\delta = 0$ in Claim 1, we can get that there exists a neural network $\phi_{\text{score}}(w, x, t) \in \Phi(H, W, R, B, V)$ with $H = \Theta\big(\log^4 n\big)$, $\|W\|_\infty = \widetilde{\Theta}\big(n^{\frac{d_X}{2\alpha_X + d_X}}\big)$, $R = \widetilde{\Theta}\big(n^{\frac{d_X}{2\alpha_X + d_X}}\big)$, $B = \exp\big(\Theta(\log^4 n)\big)$ and $V = \Theta(\sqrt{\frac{\log n}{\underline{t} \wedge 1}})$ so that for any $t \in [\underline{t}, \overline{t}]$ and $(x, w) \in \{x \in \mathcal{M}_X, w \in \mathbb{R}^{D_Y} : \mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0 \sigma_{\underline{t}} \sqrt{\log n}\}$,

$$\|\phi_{\text{score}}(w, x, t) - \nabla \log p_{t|x}(w)\|_\infty = \widetilde{\mathcal{O}}(\varepsilon_2^{\alpha_X}).$$

So by Lemma C.4, we have

$$\mathbb{E}_{\mu_X^*}\Big[\int_{\underline{t}}^{\overline{t}} \int_{\mathbb{R}^{D_Y}} \big\|\phi_{\text{score}}(w, x, t) - \nabla \log p_{t|x}(w)\big\|^2 p_{t|x}(w)\, \mathrm{d}w\mathrm{d}t\Big] = \widetilde{\mathcal{O}}(n^{-\frac{2\alpha_X}{2\alpha_X + d_X}}).$$

Now we show Claim 1. Recall $\mathcal{K}_{\widetilde{x}} = \{k \in [K] : \|\widetilde{x} - x_k^*\| \le 2r\}$. Then consider $\varepsilon_1 = c_1 n^{-\delta}(\log n)^{-1}$ and let $\mathcal{N}_{\varepsilon_1}^Z = \{\widetilde{z}_1, \widetilde{z}_2, \cdots, \widetilde{z}_{J_1}\}$ be one of the largest ε_1-packing of $\mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$, where $\overline{r}$ is the positive constant required in Lemma C.5. We have $|J_1| \lesssim \varepsilon_1^{-d_Y}$. Then we define

$$\mathcal{N} = \{(\widetilde{x}, y) : y = G_{[k]}^*(z, \widetilde{x}), k \in \mathcal{K}_{\widetilde{x}}, z \in \mathcal{N}_{\varepsilon_1}^Z\}.$$

For any $(x, y) \in \mathcal{M}$ so that $\|x - \widetilde{x}\| \le \varepsilon_2 < r$, since $\{(x_k^*, y_k^*)\}_{k=1}^K$ is an r-cover of $\mathcal{M}$, there exists $k \in \mathcal{K}_{\widetilde{x}}$ so that $\|x - x_k^*\| \le r$ and $\|y - y_k^*\| \le r$. So by lemma C.5, it holds that $Q_{[k]}^*(y, x) \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$ and there exists $z \in \mathcal{N}_{\varepsilon_1}^Z$ so that $\|z - Q_{[k]}^*(y, x)\| \le \varepsilon_1$. Thus,

$$\begin{aligned}
\|y - G_{[k]}^*(z, \widetilde{x})\| &= \|G_{[k]}^*(Q_{[k]}^*(y, x), x) - G_{[k]}^*(z, \widetilde{x})\| \\
&\le \|G_{[k]}^*(Q_{[k]}^*(y, x), x) - G_{[k]}^*(z, x)\| + \|G_{[k]}^*(z, x) - G_{[k]}^*(z, \widetilde{x})\| \\
&\le C\varepsilon_1.
\end{aligned} \tag{3}$$

Then let $J := |\mathcal{N}|$ and write $\mathcal{N} = (\omega_1 = (\widetilde{x}, y_1), \omega_2 = (\widetilde{x}, y_2), \cdots, \omega_J = (\widetilde{x}, y_J))$, we have for any $x \in \mathbb{B}_{\mathcal{M}_X}(\widetilde{x}, \varepsilon_2)$ and $y \in \mathcal{M}_{Y|x}$, there exists $\omega_j = (\widetilde{x}, y_j)$ so that $\|y - y_j\| \le C\varepsilon_1$. So we consider a partition of unity $\widetilde{\rho}_j(\cdot) = \rho_j(\cdot)/\sum_{j=1}^J \rho_j(\cdot)$ with

$$\rho_j(y) = \rho(\frac{\|y - y_j\|^2}{C^2 \varepsilon_1^2})$$

and ρ is the following smooth transition function

$$\rho(t) = \begin{cases} 0 & |t| \ge 2 \\ 1 & |t| \le 1 \\ \frac{1}{1 + \exp(\frac{2x - 3}{x^2 - 3x + 2})} & 1 < t < 2 \\ \frac{1}{1 + \exp(\frac{-2x - 3}{x^2 + 3x + 2})} & -2 < t < -1. \end{cases} \tag{4}$$

Then for any $x \in \mathbb{B}_{\mathcal{M}_X}(\widetilde{x}, \varepsilon_2)$ and $w \in \mathbb{R}^{D_Y}$ so that $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0 \sigma_{\underline{t}} \sqrt{\log n}$, by Lemma B.2, we have

$$
\begin{aligned}
&\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot - \frac{(w-m_t y)}{\sigma_t}\right] \\
&= \sum_{j=1}^{J} \mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\widetilde{\rho}_j(y)\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot - \frac{(w-m_t y)}{\sigma_t}\right] \\
&= \sum_{j=1}^{J} \mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\widetilde{\rho}_j(y)\mathbf{1}(y\in\mathbb{B}_{\mathcal{M}_{Y|x}}(y_j,\sqrt{2}C\varepsilon_1))\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot - \frac{(w-m_t y)}{\sigma_t}\right] \\
&= \sum_{j\in[J]}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} \exp\left(-\frac{\|w-m_t G^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\cdot - \frac{(w-m_t G^{\omega_j}(z,x))}{\sigma_t}\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z.
\end{aligned}
$$

Then notice that for any $(x, y) \in \mathcal{M}$ so that $\|x - \widetilde{x}\| \le \varepsilon_2$ and $\widetilde{\rho}_j(y) \ne 0$,

$$
\begin{aligned}
&\|G^{\omega_j}(0,x) - y\| \\
&\le \|G^{\omega_j}(0,x) - y_j\| + \|y_j - y\| \\
&= \|G^{\omega_j}(0,x) - G^{\omega_j}(0,\widetilde{x})\| + \|y_j - y\| \\
&\lesssim \varepsilon_1 + \varepsilon_2^{\beta_X\wedge 1},
\end{aligned}
$$

and thus

$$
\|Q_x^{\omega_j}(y)\| = \|Q_x^{\omega_j}(y) - Q_x^{\omega_j}(G^{\omega_j}(0,x))\| \lesssim \varepsilon_1 + \varepsilon_2^{\beta_X\wedge 1} \lesssim \varepsilon_1.
$$

So we have

$$
\begin{aligned}
&\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot - \frac{(w-m_t y)}{\sigma_t}\right] \\
&= \sum_{j\in[J]}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|w-m_t G^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\cdot - \frac{(w-m_t G^{\omega_j}(z,x))}{\sigma_t}\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z.
\end{aligned}
$$

Notice that $G^{\omega_j}(z, x)$ is $C^{\beta_Y,\beta_X}_{D_Y}$-smooth, let

$$
G^{\omega_j}|_{\widetilde{x}}(z,x) = \sum_{\substack{j_1\in\mathbb{N}_0^{D_X} \\ |j_1|<\beta_X}} \frac{G^{\omega_j}_{(0_{d_Y},j_1)}(z,\widetilde{x})}{j_1!}(x-\widetilde{x})^{j_1},
$$

we have

$$
\|G^{\omega_j}(z,x) - G^{\omega_j}|_{\widetilde{x}}(z,x)\| \lesssim \|x-\widetilde{x}\|^{\beta_X} \lesssim \varepsilon_2^{\beta_X}.
$$

So based on the decomposition

$$
\begin{aligned}
\|w - m_t G^{\omega_j}(z,x)\|^2 = \|w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x)\|^2 &+ 2\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}(z,x)\rangle \\
&+ \|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}(z,x)\|^2,
\end{aligned}
$$

we can obtain

$$
\begin{aligned}
&\sum_{j\in[J]}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|w-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w-m_tG^{\omega_j}(z,x))}{\sigma_t}\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z\\
&=\sum_{j\in[J]}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x), m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot -\frac{(w-m_tG^{\omega_j}(z,x))}{\sigma_t}\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z\cdot\exp\left(-\frac{\|w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x)\|^2}{2\sigma_t^2}\right).
\end{aligned}
$$

Similarly, we have

$$
\begin{aligned}
&\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\right]\\
&=\sum_{j\in[J]}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|w-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z\\
&=\sum_{j\in[J]}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x), m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z\cdot\exp\left(-\frac{\|w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x)\|^2}{2\sigma_t^2}\right).
\end{aligned}
$$

Notice that for any $j\in[J]$, $x\in\mathbb{B}_{\mathcal{M}_X}(\widetilde{x},\varepsilon_2)$, $w\in\mathbb{R}^{D_Y}$ with $\mathrm{dist}(w,\mathcal{M}_{Y|x})\le c_0\sigma_{\underline{t}}\sqrt{\log n}$ and $t\in[\underline{t},\overline{t}]$, we have

$$
\frac{\|w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x)\|^2}{2\sigma_t^2}\lesssim\log n,
$$

and for any $\|z\|\lesssim\varepsilon_1$,

$$
\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\lesssim\frac{\varepsilon_1^2+\varepsilon_2^{2\beta_X}}{\sigma_t^2}\lesssim\frac{\varepsilon_1^2}{\sigma_t^2}=\mathcal{O}(1),
$$

and

$$
\left|\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x), m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\rangle}{\sigma_t^2}\right|=\mathcal{O}(\frac{\varepsilon_1}{\sigma_{\underline{t}}}\sqrt{\log n})=\mathcal{O}(1). \tag{5}
$$

Moreover, there exists a small enough constant c so that when $\|z\|\le c\varepsilon_1$,

$$
\|G^{\omega_j}(z,x)-y_j\|=\|G^{\omega_j}(z,x)-G^{\omega_j}(0,\widetilde{x})\|\le C\varepsilon_1,
$$

which implies that $\widetilde{\rho}_j(G^{\omega_j}(z,x))$ is bounded away from zero. We can then obtain

$$
\begin{aligned}
&\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\quad\cdot\exp\left(-\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x), m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\rangle}{\sigma_t^2}\right)\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z\asymp\varepsilon_1^{d_Y},
\end{aligned}
$$

$$
\left\|\frac{w-m_tG^{\omega_j}|_{\widetilde{x}}(z,x)}{\sigma_t}\right\|\lesssim\sqrt{\log n},
$$

and

$$\exp\left(-\frac{\|w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x)\|^2}{2\sigma_t^2}\right)\gtrsim n^{-C_1},$$

for some positive constant C_1. Therefore, if for any $j\in[J]$, there exist neural networks $\phi_j^{[1]}(w,x,t)$, $\phi_j^{[2]}(w,x,t)$ and $\phi_j^{[3]}(w,x,t)$ and number $\epsilon=o(1)$ so that for any $x\in\mathbb{B}_{\mathcal{M}_X}(\widetilde{x},\varepsilon_2)$, $w\in\mathbb{R}^{D_Y}$ with $\mathrm{dist}(w,\mathcal{M}_{Y|x})\le c_0\sigma_{\underline{t}}\sqrt{\log n}$ and $t\in[\underline{t},\overline{t}]$,

$$\begin{aligned}&\Bigg\|\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)}\exp\left(-\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\\&\cdot\exp\left(-\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x),m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\rangle}{\sigma_t^2}\right)\\&\cdot-\frac{(w-m_tG^{\omega_j}(z,x))}{\sigma_t}\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z-\phi_j^{[1]}(w,x,t)\Bigg\|_\infty\lesssim\varepsilon_1^{-d_Y}\epsilon\sqrt{\log n},\end{aligned}\tag{6}$$

$$\begin{aligned}&\Bigg|\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)}\exp\left(-\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right)\\&\cdot\exp\left(-\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x),m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\rangle}{\sigma_t^2}\right)\widetilde{\rho}_j(G^{\omega_j}(z,x))v^{\omega_j}(z|x)\,\mathrm{d}z\\&\quad-\phi_j^{[2]}(w,x,t)\Bigg|\lesssim\varepsilon_1^{-d_Y}\epsilon,\end{aligned}\tag{7}$$

and

$$\left|\exp\left(-\frac{\|w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x)\|^2}{2\sigma_t^2}\right)-\phi_j^{[3]}(w,x,t)\right|\lesssim n^{-C_1}\epsilon.\tag{8}$$

Then it holds that

$$\left\|\nabla\log p_{t|x}(w)-\frac{1}{\sigma_t}\cdot\frac{\sum_{j=1}^J\phi_j^{[1]}(w,x,t)\phi_j^{[3]}(w,x,t)}{\sum_{j=1}^J\phi_j^{[2]}(w,x,t)\phi_j^{[3]}(w,x,t)}\right\|_\infty\lesssim\log n\cdot\epsilon.\tag{9}$$

Now we build such neural networks. Notice that $v^{\omega_j}(z|x)$ is C^{α_Y,α_X}-smooth, let

$$v^{\omega_j}|_{\widetilde{x}}(z|x)=\sum_{\substack{j_1\in\mathbb{N}_0^{D_X}\\|j_1|<\alpha_X}}\frac{v^{\omega_j}_{(0,j_1)}(z|\widetilde{x})}{j_1!}(x-\widetilde{x})^{j_1},$$

we have

$$\|v^{\omega_j}(z|x)-v^{\omega_j}|_{\widetilde{x}}(z|x)\|\lesssim\|x-\widetilde{x}\|^{\alpha_X}\lesssim\varepsilon_2^{\alpha_X}.$$

Furthermore, for any $x\in\mathbb{B}_{\mathcal{M}_X}(\widetilde{x},\varepsilon_2)$, $z\in\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)$ and $w\in\mathbb{R}^{D_Y}$ with $\mathrm{dist}(w,\mathcal{M}_{Y|x})\le c_0\sigma_{\underline{t}}\sqrt{\log n}$, it holds that

$$\left|\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\|^2}{2\sigma_t^2}-\frac{\|m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right|\lesssim\log n\cdot\varepsilon_1\cdot\varepsilon_2^{\beta_X};$$

$$\begin{aligned}&\Bigg|\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x),m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}(z,x)\rangle}{\sigma_t^2}\\&-\frac{\langle w-m_tG^{\omega_j}|_{\widetilde{x}}(0,x),m_tG^{\omega_j}|_{\widetilde{x}}(0,x)-m_tG^{\omega_j}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\Bigg|\lesssim\log n\cdot\varepsilon_2^{\beta_X}\end{aligned}$$

$$\left\|\frac{(w-m_tG^{\omega_j}(z,x))}{\sigma_t}-\frac{(w-m_tG^{\omega_j}|_{\widetilde{x}}(z,x))}{\sigma_t}\right\|\lesssim\sqrt{\log n}\cdot\varepsilon_2^{\beta_X}.$$

Moreover, by equation (3), for any $z \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, C_1\varepsilon_1)$, $x \in \mathbb{B}_{\mathcal{M}_X}(\widetilde{x}, \varepsilon_2)$ and $j \in [J]$,

$$\sum_{k=1}^{J} \rho_k(G^{\omega_j}(z,x)) \geq 1.$$

So we have

$$\begin{aligned}
&\left|\widetilde{\rho}_j(G^{\omega_j}(z,x)) - \widetilde{\rho}_j(G^{\omega_j}|_{\widetilde{x}}(z,x))\right| \\
&\leq \left|\frac{\rho_j(G^{\omega_j}(z,x))}{\sum_{k=1}^J \rho_k(G^{\omega_j}(z,x))} - \frac{\rho_j(G^{\omega_j}|_{\widetilde{x}}(z,x))}{\sum_{k=1}^J \rho_k(G^{\omega_j}(z,x))}\right| + \left|\frac{\rho_j(G^{\omega_j}|_{\widetilde{x}}(z,x))}{\sum_{k=1}^J \rho_k(G^{\omega_j}(z,x))} - \frac{\rho_j(G^{\omega_j}|_{\widetilde{x}}(z,x))}{\sum_{k=1}^J \rho_k(G^{\omega_j}|_{\widetilde{x}}(z,x))}\right| \\
&\lesssim \frac{\varepsilon_2^{\beta_X}}{\varepsilon_1}.
\end{aligned}$$

Then for any $z \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, C_1\varepsilon_1)$, denote $\widetilde{\rho}_j^z(x) = \widetilde{\rho}_j(G^{\omega_j}|_{\widetilde{x}}(z,x))$ as a function of x, $\widetilde{\rho}_j^z(\cdot)$ is C^∞ around $\widetilde{x}$ with $|\widetilde{\rho}_j^{z\,(j_1)}(\widetilde{x})| \lesssim \varepsilon_1^{-|j_1|}$. So set $\delta_1 = \lceil \frac{\beta_X \log \varepsilon_2}{\log \varepsilon_2 - \log \varepsilon_1} \rceil \leq \lceil 2\beta_X \rceil$, we have

$$\widetilde{\rho}_j(G^{\omega_j}|_{\widetilde{x}}(z,x)) = \widetilde{\rho}_j^z(x) = \sum_{\substack{j_1 \in \mathbb{N}_0^{D_X} \\ |j_1| < \delta_1}} \frac{\widetilde{\rho}_j^{z\,(j_1)}(\widetilde{x})}{j_1!}(x - \widetilde{x})^{j_1} + O(\varepsilon_2^{\beta_X}).$$

Then denote

$$\widetilde{\rho}_j^z|_{\widetilde{x}}(x) = \sum_{\substack{j_1 \in \mathbb{N}_0^{D_X} \\ |j_1| < \delta_1}} \frac{\widetilde{\rho}_j^{z\,(j_1)}(\widetilde{x})}{j_1!}(x - \widetilde{x})^{j_1}.$$

By combining all pieces, we can obtain

$$\begin{aligned}
&\Big\| \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\cdot \exp\left(-\frac{\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}(z,x)\rangle}{\sigma_t^2}\right) \\
&\cdot -\frac{(w - m_t G^{\omega_j}(z,x))}{\sigma_t} \widetilde{\rho}_j(G^{\omega_j}(z,x)) v^{\omega_j}(z|x)\, \mathrm{d}z \\
&- \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\cdot \exp\left(-\frac{\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\right) \\
&\cdot -\frac{(w - m_t G^{\omega_j}|_{\widetilde{x}}(z,x))}{\sigma_t} \widetilde{\rho}_j^z|_{\widetilde{x}}(x) v^{\omega_j}|_{\widetilde{x}}(z|x)\, \mathrm{d}z \Big\| \\
&\lesssim \sqrt{\log n} \cdot \varepsilon_1^{-d_Y - 1} \varepsilon_2^{\beta_X} + \sqrt{\log n} \cdot \varepsilon_1^{-d_Y} \varepsilon_2^{\alpha_X} \\
&\lesssim \sqrt{\log n} \cdot \varepsilon_1^{-d_Y} \varepsilon_2^{\alpha_X},
\end{aligned}$$

where the last inqulity uses $\varepsilon_1 \geq \varepsilon_2^{\frac{\alpha_X}{\alpha_Y} \wedge \frac{1}{2}} \geq \varepsilon_2^{\frac{\alpha_X}{\alpha_Y}} = \varepsilon_2^{\beta_X - \alpha_X}$. Since for any $-1 < z < 1$, we have $|\exp(z) - \sum_{l=0}^{\mathscr{L}} \frac{z^l}{l!}| \leq e\frac{|z|^{\mathscr{L}+1}}{(\mathscr{L}+1)!} \leq e(\frac{|z|e}{\mathscr{L}+1})^{\mathscr{L}+1}$. Set $\mathscr{L}_1 = \frac{\alpha_X \log \varepsilon_2}{\log(\varepsilon_1^2) - \log(\sigma_{\underline{t}}^2)}$ and $\mathscr{L}_2 = \frac{\alpha_X \log \varepsilon_2}{\log(\varepsilon_1 \sqrt{\log n}) - \log(\sigma_{\underline{t}})}$, using inequality (5), we have

$$\begin{aligned}
&\Bigg| \exp\left(-\frac{\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\right) \\
&- \sum_{l=0}^{\mathscr{L}_2} (-1)^l \frac{\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\rangle^l}{l!(\sigma_t)^{2l}} \Bigg| \lesssim \varepsilon_2^{\alpha_X}.
\end{aligned}$$

$$\left| \exp\left(-\frac{\|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right) - \sum_{l=0}^{\mathscr{L}_1} (-1)^l \frac{\|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\|^{2l}}{2^l l!(\sigma_t)^{2l}} \right| \lesssim \varepsilon_2^{\alpha_X}.$$

Therefore,

$$\begin{aligned}
&\Bigg\| \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \exp\left(-\frac{\|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\quad\cdot \exp\left(-\frac{\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\right) \\
&\quad\cdot -\frac{(w - m_t G^{\omega_j}|_{\widetilde{x}}(z,x))}{\sigma_t} \widetilde{\rho}_j^z|_{\widetilde{x}}(x) v^{\omega_j}|_{\widetilde{x}}(z|x)\,\mathrm{d}z \\
&- \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \sum_{l=0}^{\mathscr{L}_1} (-1)^l \frac{\|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\|^{2l}}{l!(\sigma_t)^{2l}} \\
&\quad\cdot \sum_{l=0}^{\mathscr{L}_2} (-1)^l \frac{\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\rangle^l}{l!(\sigma_t)^{2l}} \\
&\quad\cdot -\frac{(w - m_t G^{\omega_j}|_{\widetilde{x}}(z,x))}{\sigma_t} \widetilde{\rho}_j^z|_{\widetilde{x}}(x) v^{\omega_j}|_{\widetilde{x}}(z|x)\,\mathrm{d}z \Bigg\|_\infty \\
&\lesssim \varepsilon_2^{\alpha_X} \varepsilon_1^{-d} \sqrt{\log n}.
\end{aligned}$$

Notice that we can write

$$\begin{aligned}
&\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C_1\varepsilon_1)} \sum_{l=0}^{\mathscr{L}_1} (-1)^l \frac{\|m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\|^{2l}}{2^l l!(\sigma_t)^{2l}} \\
&\quad\cdot \sum_{l=0}^{\mathscr{L}_2} (-1)^l \frac{\langle w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x), m_t G^{\omega_j}|_{\widetilde{x}}(0,x) - m_t G^{\omega_j}|_{\widetilde{x}}(z,x)\rangle^l}{l!(\sigma_t)^{2l}} \\
&\quad\cdot -\frac{(w - m_t G^{\omega_j}|_{\widetilde{x}}(z,x))}{\sigma_t} \widetilde{\rho}_j^z|_{\widetilde{x}}(x) v^{\omega_j}|_{\widetilde{x}}(z|x)\,\mathrm{d}z \\
&= \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,C\varepsilon_1)} \sum_{l=0}^{\mathscr{L}_1} \frac{(-1)^l m_t^{2l}}{2^l l!(\sigma_t)^{2l}} \Bigg\| \sum_{j_1\in\mathbb{N}_0^{D_X}, |j_1|<\beta_X} (G^{\omega_j}_{(0,j_1)}(0,\widetilde{x}) - G^{\omega_j}_{(0,j_1)}(z,\widetilde{x})) \frac{(x-\widetilde{x})^{j_1}}{j_1!} \Bigg\|^{2l} \\
&\cdot \sum_{l=0}^{\mathscr{L}_2} \frac{(-1)^l m_t^l}{l!(\sigma_t)^{2l}} \left\langle w - m_t \sum_{j_1\in\mathbb{N}_0^{D_X}, |j_1|<\beta_X} G^{\omega_j}_{(0,j_1)}(0,\widetilde{x}) \frac{(x-\widetilde{x})^{j_1}}{j_1!}, \sum_{j_1\in\mathbb{N}_0^{D_X}, |j_1|<\beta_X} (G^{\omega_j}_{(0,j_1)}(0,\widetilde{x}) - G^{\omega_j}_{(0,j_1)}(z,\widetilde{x})) \frac{(x-\widetilde{x})^{j_1}}{j_1!} \right\rangle^l \\
&\cdot -\frac{w - m_t \sum_{j_1\in\mathbb{N}_0^{D_X}, |j_1|<\beta_X} G^{\omega_j}_{(0,j_1)}(z,\widetilde{x}) \frac{(x-\widetilde{x})^{j_1}}{j_1!}}{\sigma_t} \cdot \sum_{j_1\in\mathbb{N}_0^{D_X}, |j_1|<\delta_1} \frac{\widetilde{\rho}_j^{z\,(j_1)}(\widetilde{x})}{j_1!} (x-\widetilde{x})^{j_1} \cdot \sum_{j_1\in\mathbb{N}_0^{D_X}, |j_1|<\alpha_X} \frac{v^{\omega_j}_{(0,j_1)}(z|\widetilde{x})}{j_1!} (x-\widetilde{x})^{j_1}\,\mathrm{d}z \\
&= \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} (\frac{1}{\sigma_t})^{2l_1+2l_2+1} \sum_{0\le k\le 2l_1+2l_2+1} m_t^k \sum_{i\in\mathbb{N}_0^{D_Y}, |i|\le l_2+1} w^{(i)} \sum_{s\in\mathbb{N}_0^{D_X}, |s|\le(2l_1+2l_2+1)\lfloor\beta_X\rfloor+\lfloor\delta_1\rfloor+\lfloor\alpha_X\rfloor} a_{l_1 l_2 k i l} \cdot x^{(s)},
\end{aligned}$$

where $a_{l_1 l_2 k i l} \in \mathbb{R}^{D_Y}$ and $(\frac{1}{\sigma_t})^{2l_1+2l_2+1} a_{l_1 l_2 k i l} \lesssim \exp(\mathcal{O}(\log^2 n))$. Therefore, using Lemmas C.7, C.8, C.9 and C.10, we

1. Approximate m_t by $\phi_m(t) \in \Phi(H, W, R, B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta(\log^6 n)$, $R = \Theta(\log^8 n)$ and $B = \exp(\Theta(\log^4 n))$.

2. Approximate σ_t by $\phi_\sigma(t) \in \Phi(H, W, R, B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta(\log^6 n)$, $R = \Theta(\log^8 n)$ and $B = \exp(\Theta(\log^4 n))$.

3. Approximate $\frac{1}{x}$ by $\phi_{rec}(x) \in \Phi(H, W, R, B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta(\log^6 n)$, $R = \Theta(\log^8 n)$ and $B = \exp(\Theta(\log^4 n))$.

4. For vector $x \in \mathbb{R}^{D_X}$, approximate $x^{(i)}$ by $\phi^{[D_X]}_{vpower}(x;i) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n \cdot \log\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log^3 n)$ and $B = \exp(\Theta(\log n))$.

5. For vector $w \in \mathbb{R}^{D_Y}$, approximate $w^{(i)}$ by $\phi^{[D_Y]}_{vpower}(w;i) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n \cdot \log\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log^3 n)$ and $B = \exp(\Theta(\log n \cdot \log\log n))$.

6. For $x \in \mathbb{R}$, Approximate x^a by $\phi_{power}(x;a) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n \log\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log^3 n)$ and $B = \exp(\Theta(\log n \cdot \log\log n)$.

7. For $x, y \in \mathbb{R}$, Approximate $x \cdot y$ by $\phi_{mult}(x,y) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n)$, $\|W\|_\infty = \Theta(1)$, $R = \Theta(\log^2 n)$ and $B = \exp(\Theta(\log^2 n))$.

We have for any $x \in \mathbb{B}_{\mathcal{M}_X}(\widetilde{x}, \varepsilon_2)$, $w \in \mathbb{R}^{D_Y}$ with $\operatorname{dist}(w, \mathcal{M}_{Y|x}) \le c_0 \sigma_{\underline{t}} \sqrt{\log n}$ and $t \in [\underline{t}, \overline{t}]$,

$$\Bigg\| \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} \Big(\frac{1}{\sigma_t}\Big)^{2l_1+2l_2+1} \sum_{0 \le k \le 2l_1+2l_2+1} m_t^k \sum_{i \in \mathbb{N}_0^{D_Y}, |i| \le l_2+1} w^{(i)} \sum_{s \in \mathbb{N}_0^{D_X}, |s| \le (2l_1+2l_2+1)\lfloor \beta_X \rfloor + \lfloor \delta_1 \rfloor + \lfloor \alpha_X \rfloor} a_{l_1 l_2 kil} \cdot x^{(s)}$$
$$- \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} \sum_{0 \le k \le 2l_1+2l_2+1} \sum_{i \in \mathbb{N}_0^{D_Y}, |i| \le l_2+1} \sum_{s \in \mathbb{N}_0^{D_X}, |s| \le (2l_1+2l_2+1)\lfloor \beta_X \rfloor + \lfloor \delta_1 \rfloor + \lfloor \alpha_X \rfloor} a_{l_1 l_2 kil}$$
$$\cdot \phi_{mult}\bigg(\phi_{mult}\Big(\phi_{mult}\Big(\phi_{power}\big(\phi_{rec}(\phi_\sigma(t)); 2l_1+2l_2+1\big), \phi_{power}\big(\phi_m(t); k\big)\Big), \phi^{[D_Y]}_{vpower}(\omega; i)\Big), \phi^{[D_X]}_{vpower}(x; s)\bigg)\Bigg\|_\infty$$
$$\lesssim \varepsilon_2^{\alpha_X} \varepsilon_1^{-d} \sqrt{\log n}.$$

Therefore, based on Lemmas F.1-F.3 in [2] for the concatenation and parallelization of neural networks, let $\mathscr{L} = \mathscr{L}_1 \mathscr{L}_2 \cdot (2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\binom{\mathscr{L}_2 + D_Y}{D_Y}\binom{(2\mathscr{L}_1+2\mathscr{L}_2+1)\lfloor \beta_X \rfloor + \delta_1 + \lfloor \alpha_X \rfloor + D_X}{D_X}$, there exists networks $\phi_j^{[1]}(w,x,t) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta\big(\log^6 n \mathscr{L}\big)$, $R = \Theta\big(\log^8 n \mathscr{L}\big)$, $B = \exp(\Theta(\log^4 n))$ so that (6) holds with $\epsilon = \mathcal{O}(\varepsilon_2^{\alpha_X})$. Similarly, there exists a neural network $\phi_j^{[2]}(w,x,t)$ with the same size as $\phi_j^{[1]}(w,x,t)$ so that (7) holds with $\epsilon = \mathcal{O}(\varepsilon_2^{\alpha_X})$. For the term $\exp\Big(-\frac{\|w - m_t G^{\omega_j}|_{\widetilde{x}}(0,x)\|^2}{2\sigma_t^2}\Big)$, using Lemmas C.7-C.10, there exists $\phi_j^{[3]}(w,x,t) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta(\log^6 n)$, $R = \Theta(\log^8 n)$, $B = \exp(\Theta(\log^4 n))$ so that (8) holds with $\epsilon = \mathcal{O}(\varepsilon_2^{\alpha_X})$. Then using (9) and Lemmas C.4, C.9, C.10, we can obtain

$$\Bigg\| \max\Bigg\{ \frac{-c_2\sqrt{\log n}}{\sigma_{\underline{t}}}, \min\Bigg\{ \frac{c_2\sqrt{\log n}}{\sigma_{\underline{t}}}, \phi_{mult}\bigg(\phi_{rec}\left(\phi_\sigma(t)\right), \phi_{mult}\Big(\sum_{j=1}^{J} \phi_j^{[1]}(w,x,t)\phi_j^{[3]}(w,x,t),$$
$$\phi_{rec}\big(\sum_{j=1}^{J} \phi_j^{[2]}(w,x,t)\phi_j^{[3]}(w,x,t)\big)\Big)\bigg)\Bigg\}\Bigg\} - \nabla \log p_{t|x}(w) \Bigg\|_\infty = \mathcal{O}(\log n \cdot \varepsilon_2^{\alpha_X}).$$

The desired result then follows from Lemmas F.1-F.3 in [2] for the concatenation and parallelization of neural networks.

Remark C.1. *Here, choosing* $\varepsilon_1 = (\log n)^{-1}$ *will result in a factor of* $(\log n)^{D_Y}$ *due to the orders of* $\mathscr{L}_1$ *and* $\mathscr{L}_2$ *being* $\Theta(\log n)$*. This can lead to problems when* D_Y *is significantly large. To address this issue, we can instead choose* $\varepsilon_1 = n^{-\delta}(\log n)^{-1}$*, where* $\delta > 0$ *is a small number. With this choice,* $\mathscr{L}_1$ *and* $\mathscr{L}_2$ *will be of constant order, and the influence on the neural network size will be* $\mathcal{O}(n^{\delta d_Y})$.

C.1.2 Case 2: $c' n^{-2\delta}(\log n)^{-3} \le \underline{t} \le c \log^{-1} n$ with $0 \le \delta < \frac{\frac{\alpha_X}{\alpha_Y} \wedge \frac{1}{2}}{2\alpha_X + d_X}$ and c' is a small enough positive constant

Set $\varepsilon_1 = \sigma_{\underline{t}}\sqrt{\log n}$ and $\varepsilon_2 = n^{-\frac{1}{2\alpha_X + d_X}}$. Let $\mathcal{N}^X_{\varepsilon_2}$ be one of the largest ε_2-packing of $\mathcal{M}_X$ and $\mathcal{N}^Z_{\varepsilon_1}$ be one of the largest ε_1-packing of $\mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$. Then we have $J_1 := |\mathcal{N}^Z_{\varepsilon_1}| \lesssim \varepsilon_1^{-d_Y}$ and $J_2 := |\mathcal{N}^X_{\varepsilon_2}| \lesssim$

$\varepsilon_2^{-d_X}$. Now we take an arbitrary $\widetilde{x} \in \mathcal{N}^X_{\varepsilon_2}$, $k \in \mathcal{K}_{\widetilde{x}} = \{k \in [K] : \|\widetilde{x} - x^*_k\| \le 2r\}$ and $\widetilde{z} \in N^Z_{\varepsilon_1}$, consider set

$$\mathscr{S}_{k\widetilde{x}\widetilde{z}} = \Big\{(x, w) : x \in \mathbb{B}_{\mathcal{M}_X}(\widetilde{x}, \sqrt{2}\varepsilon_2), w \in \mathbb{R}^{D_Y}, \\ \|w - G^*_{[k]}(\widetilde{z}, x)\| \le C\,\sigma_{\underline{t}}\sqrt{\log n}, \mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}\},$$

we claim that

Claim 2. *For any* $0 \le \delta < \frac{\frac{\alpha_X}{\alpha_Y}\wedge\frac{1}{2}}{2\alpha_X + d_X}$, *let* $\widetilde{\varepsilon}_1 = c_1\,\sigma_{\underline{t}}\frac{n^{-\delta}}{\sqrt{\log n}}$, $\mathscr{L}_1 = \frac{\alpha_X \log\varepsilon_2}{\log(\widetilde{\varepsilon}_1^2) - \log(\sigma^2_{\underline{t}})}$, $\mathscr{L}_2 = \frac{\alpha_X\log\varepsilon_2}{\log(\varepsilon_1\sqrt{\log n}) - \log(\sigma_{\underline{t}})}$ *and* $\mathscr{L} = \mathscr{L}_1\mathscr{L}_2\cdot(2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\binom{\mathscr{L}_2 + D_Y}{D_Y}\binom{(2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\lfloor\beta_X\rfloor + \lfloor\alpha_X\rfloor + D_X}{D_X}$, *then when* c_1 *is small enough, there exist a network* $\phi^*(w, x, t) \in \Phi\big(H, W, R, B, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ *with* $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta\big(\log^6 n\mathscr{L}(\frac{\varepsilon_1}{\widetilde{\varepsilon}_1})^{d_Y}\big)$, $R = \Theta\big(\log^8 n\mathscr{L}(\frac{\varepsilon_1}{\widetilde{\varepsilon}_1})^{d_Y}\big)$, $B = \exp(\Theta(\log^4 n))$, *so that for any* $(x, w) \in \mathscr{S}_{k\widetilde{x}\widetilde{z}}$, *and* $t \in [\underline{t}, \overline{t}]$,

$$\|\phi^*(w, x, t) - \nabla\log p_{t|x}(w)\|_\infty = \mathcal{O}(\varepsilon_2^{\alpha_X}\log n).$$

Then similar as Case 1, by setting $\delta = 0$, using Lemmas C.4 and C.6, we can get that there exists a neural network $\phi_{\text{score}}(w, x, t) \in \Phi(H, W, R, B, V)$ with $H = \Theta\big(\log^4 n\big)$, $\|W\|_\infty = \widetilde{\Theta}\big(n^{\frac{d_X}{2\alpha_X + d_X}}\big)$, $R = \widetilde{\Theta}\big(n^{\frac{d_X}{2\alpha_X + d_X}}\big)$, $B = \exp\big(\Theta(\log^4 n)\big)$ and $V = \Theta(\sqrt{\frac{\log n}{\underline{t}\wedge 1}})$ so that for any $t \in [\underline{t}, \overline{t}]$ and $(x, w) \in \{x \in \mathcal{M}_X, w \in \mathbb{R}^{D_Y} : \mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}\}$,

$$\mathbb{E}_{\mu^*_X}\Big[\int_{\underline{t}}^{\overline{t}}\int_{\mathbb{R}^{D_Y}}\big\|\phi_{\text{score}}(w, x, t) - \nabla\log p_{t|x}(w)\big\|^2 p_{t|x}(w)\,\mathrm{d}w\mathrm{d}t\Big] = \widetilde{\mathcal{O}}(n^{-\frac{2\alpha_X}{2\alpha_X + d_X}}).$$

By combining the result from Case 1, we can deduce the third statement in Lemma C.2.

Now we show Claim 2. When $t \le c\log^{-1} n$ for a small enough c, we have for any $(x, w) \in \mathscr{S}_{k\widetilde{x}\widetilde{z}}$,

$$\begin{aligned}&\{y \in \mathcal{M}_{Y|x} : \|y - w\| \le c_2\sigma_{\underline{t}}\sqrt{\log n}\}\\ &\subset \{y \in \mathcal{M}_{Y|x} : \|y - G^*_{[k]}(\widetilde{z}, x)\| \le c_3\sigma_{\underline{t}}\sqrt{\log n}\}\\ &\subset \{y = G^*_{[k]}(z, x) : \|z - \widetilde{z}\| \le c_4\varepsilon_1\}.\end{aligned}$$

Let $\widetilde{\varepsilon}_1 = c_1\,\sigma_{\underline{t}}\frac{n^{-\delta}}{\sqrt{\log n}}$ and let $\overline{\mathcal{N}}^{\widetilde{z}}_{\widetilde{\varepsilon}_1} = \{\overline{z}_1, \overline{z}_2, \cdots, \overline{z}_J\}$ be one of the largest $\widetilde{\varepsilon}_1$-packing of $\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z}, c_4\varepsilon_1)$, we have $|J| = |\overline{\mathcal{N}}^{\widetilde{z}}_{\widetilde{\varepsilon}_1}| \lesssim (\frac{\widetilde{\varepsilon}_1}{\varepsilon_1})^{-d_Y}$. Then we consider $\widetilde{\rho}_j(\cdot) = \rho_j(\cdot)/\sum_{j=1}^J\rho_j(\cdot)$ with

$$\rho_j(y) = \rho(\frac{\|z - \overline{z}_j\|^2}{\widetilde{\varepsilon}_1^2})$$

and ρ is the transition function defined in (4). Then for any $(x, w) \in \mathscr{S}_{k\widetilde{x}\widetilde{z}}$, by Lemma B.2, we have

$$\begin{aligned}&\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w - m_t y\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w - m_t y)}{\sigma_t}\mathbf{1}\left(y \in \{y = G^*_{[k]}(z, x) : \|z - \widetilde{z}\| \le c_4\varepsilon_1\}\right)\right]\\
&= \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z}, c_4\varepsilon_1)}\exp\left(-\frac{\left\|w - m_t G^*_{[k]}(z, x)\right\|^2}{2\sigma_t^2}\right)\cdot -\frac{\left(w - m_t G^*_{[k]}(z, x)\right)}{\sigma_t}v^*_{[k]}(z|x)\,\mathrm{d}z\\
&= \sum_{j=1}^J\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z}, c_4\varepsilon_1)}\exp\left(-\frac{\left\|w - m_t G^*_{[k]}(z, x)\right\|^2}{2\sigma_t^2}\right)\cdot -\frac{\left(w - m_t G^*_{[k]}(z, x)\right)}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}(z|x)\,\mathrm{d}z\\
&= \sum_{j=1}^J\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z}, c_4\varepsilon_1)\cap\mathbb{B}_{\mathbb{R}^{d_Y}}(\overline{z}_j, \sqrt{2}\widetilde{\varepsilon}_1)}\exp\left(-\frac{\left\|w - m_t G^*_{[k]}(z, x)\right\|^2}{2\sigma_t^2}\right)\cdot -\frac{\left(w - m_t G^*_{[k]}(z, x)\right)}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}(z|x)\,\mathrm{d}z.\end{aligned}$$

Notice that $G^*_{[k]}(z,x)$ is $C^{\beta_Y,\beta_X}_{D_Y}$-smooth, let

$$G^*_{[k]}|_{\widetilde{x}}(z,x) = \sum_{\substack{j_1\in\mathbb{N}_0^{D_X}\\ |j_1|<\beta_X}} \frac{G^*_{[k](0,j_1)}(z,\widetilde{x})}{j_1!}(x-\widetilde{x})^{j_1},$$

we have

$$\|G^*_{[k]}(z,x) - G^*_{[k]}|_{\widetilde{x}}(z,x)\| \lesssim \|x-\widetilde{x}\|^{\beta_X} \lesssim \varepsilon_2^{\beta_X}.$$

So based on the decomposition

$$\begin{aligned}\|w - m_tG^*_{[k]}(z,x)\|^2 = \|w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)\|^2 + 2\langle w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\rangle \\ + \|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\|^2,\end{aligned}$$

we can obtain

$$\begin{aligned}&\sum_{j=1}^J \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\left\|w - m_tG^*_{[k]}(z,x)\right\|^2}{2\sigma_t^2}\right)\cdot -\frac{\left(w - m_tG^*_{[k]}(z,x)\right)}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}(z|x)\,\mathrm{d}z \\ &= \sum_{j=1}^J \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \\ &\qquad \cdot \exp\left(-\frac{\langle w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) \\ &\qquad \cdot -\frac{\left(w - m_tG^*_{[k]}(z,x)\right)}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}(z|x)\,\mathrm{d}z \cdot \exp\left(-\frac{\|w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)\|^2}{2\sigma_t^2}\right).\end{aligned}$$

Similarly, we have

$$\begin{aligned}&\sum_{j=1}^J \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\left\|w - m_tG^*_{[k]}(z,x)\right\|^2}{2\sigma_t^2}\right)\widetilde{\rho}_j(z)v^*_{[k]}(z|x)\,\mathrm{d}z \\ &= \sum_{j=1}^J \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \\ &\qquad \cdot \exp\left(-\frac{\langle w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)\widetilde{\rho}_j(z)v^*_{[k]}(z|x)\,\mathrm{d}z \\ &\qquad \cdot \exp\left(-\frac{\|w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)\|^2}{2\sigma_t^2}\right).\end{aligned}$$

Notice that for any $(x,w)\in\mathscr{S}_{k\widetilde{x}\widetilde{z}}$, $z_j\in\mathcal{N}^{\widetilde{z}}_{\widetilde{\varepsilon}_1}$, $\|z-z_j\|\le\widetilde{\varepsilon}_1$ and $t\in[\underline{t},\overline{t}]$, it holds that

$$\frac{\|w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)\|^2}{2\sigma_t^2} \le C_1\log n,$$

$$\frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2} \lesssim \frac{\widetilde{\varepsilon}_1^2}{\sigma_t^2} = \mathcal{O}(1),$$

and

$$\left|\frac{\langle w - m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right| \lesssim \frac{\widetilde{\varepsilon}_1\sqrt{\log n}}{\sigma_t} = \mathcal{O}(1).$$

Therefore, we have

$$\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \cdot \exp\left(-\frac{\langle w - m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) \widetilde{\rho}_j(z) v^*_{[k]}(z|x)\,\mathrm{d}z \asymp \widetilde{\varepsilon}_1^{d_Y},$$

$$\left|\frac{\left(w - m_t G^*_{[k]}(z,x)\right)}{\sigma_t}\right| \lesssim \sqrt{\log n},$$

and

$$\exp\left(-\frac{\|w - m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)\|^2}{2\sigma_t^2}\right) \gtrsim n^{-C_1}.$$

Therefore, if for any $j \in [J]$, there exist neural networks $\phi_j^{[1]}(w,x,t)$, $\phi_j^{[2]}(w,x,t)$ and $\phi_j^{[3]}(w,x,t)$ and number $\epsilon = o(1)$ so that for any $(x,w) \in \mathscr{S}_{k\widetilde{x}\widetilde{z}}$ and $t \in [\underline{t},\overline{t}]$,

$$\Bigg\| \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \cdot \exp\left(-\frac{\langle w - m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) \cdot -\frac{\left(w - m_t G^*_{[k]}(z,x)\right)}{\sigma_t} \widetilde{\rho}_j(z) v^*_{[k]}(z|x)\,\mathrm{d}z - \phi_j^{[1]}(w,x,t)\Bigg\|_\infty \lesssim \varepsilon_1^{-d_Y}\epsilon\sqrt{\log n}, \tag{10}$$

$$\Bigg| \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \cdot \exp\left(-\frac{\langle w - m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) \widetilde{\rho}_j(z) v^*_{[k]}(z|x)\,\mathrm{d}z - \phi_j^{[2]}(w,x,t)\Bigg| \lesssim \varepsilon_1^{-d_Y}\epsilon,$$

and

$$\left|\exp\left(-\frac{\|w - m_t G^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)\|^2}{2\sigma_t^2}\right) - \phi_j^{[3]}(w,x,t)\right| \lesssim n^{-C_1}\epsilon.$$

Then by (2), we can obtain

$$\begin{aligned} &\left\| \nabla \log p_{t|x}(w) - \frac{1}{\sigma_t} \cdot \frac{\sum_{j=1}^J \phi_j^{[1]}(w,x,t)\phi_j^{[3]}(w,x,t)}{\sum_{j=1}^J \phi_j^{[2]}(w,x,t)\phi_j^{[3]}(w,x,t)} \right\|_\infty \\ &\le \left\| \nabla \log p_{t|x}(w) - \frac{1}{\sigma_t} \cdot \frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot -\frac{(w-m_t y)}{\sigma_t} \mathbf{1}\left(y \in \{y = G^*_{[k]}(z,x) : \|z-\widetilde{z}\| \le c_4\varepsilon_1\}\right)\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mathbf{1}\left(y \in \{y = G^*_{[k]}(z,x) : \|z-\widetilde{z}\| \le c_4\varepsilon_1\}\right)\right]} \right\|_\infty \\ &+ \Bigg\| \frac{1}{\sigma_t} \cdot \frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot -\frac{(w-m_t y)}{\sigma_t} \mathbf{1}\left(y \in \{y = G^*_{[k]}(z,x) : \|z-\widetilde{z}\| \le c_4\varepsilon_1\}\right)\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mathbf{1}\left(y \in \{y = G^*_{[k]}(z,x) : \|z-\widetilde{z}\| \le c_4\varepsilon_1\}\right)\right]} \\ &\quad - \frac{1}{\sigma_t} \cdot \frac{\sum_{j=1}^J \phi_j^{[1]}(w,x,t)\phi_j^{[3]}(w,x,t)}{\sum_{j=1}^J \phi_j^{[2]}(w,x,t)\phi_j^{[3]}(w,x,t)} \Bigg\|_\infty \lesssim \frac{1}{n} + \log^2 n \cdot \epsilon. \end{aligned}$$

Now we construct such networks. Similar to Case 1, let

$$v^*_{[k]}|_{\widetilde{x}}(z,x) = \sum_{\substack{j\in\mathbb{N}_0^{d_X}\\ |j|<\alpha_X}} \frac{v^*_{[k](0,j)}(z,\widetilde{x})}{j!}(x-\widetilde{x})^j,$$

we have

$$\begin{aligned}
&\Bigg\| \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot-\frac{\Big(w-m_tG^*_{[k]}(z,x)\Big)}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}(z|x)\,\mathrm{d}z\\
&-\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot-\frac{\Big(w-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\Big)}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z\Bigg\|_\infty \lesssim \Big(\frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}}\log n+\varepsilon_2^{\alpha_X}\sqrt{\log n}\Big)\widetilde{\varepsilon}_1^{-d_Y} \lesssim \varepsilon_2^{\alpha_X}\sqrt{\log n}\,\widetilde{\varepsilon}_1^{-d_Y},
\end{aligned}$$

and by choosing $\mathscr{L}_1 = \frac{\alpha_X\log\varepsilon_2}{\log(\varepsilon_1^2)-\log(\sigma_{\underline{t}}^2)}$ and $\mathscr{L}_2 = \frac{\alpha_X\log\varepsilon_2}{\log(\varepsilon_1\sqrt{\log n})-\log(\sigma_{\underline{t}})}$,

$$\begin{aligned}
&\Bigg\| \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \exp\left(-\frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot-\frac{\Big(w-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\Big)}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z\\
&-\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \sum_{l=0}^{\mathscr{L}_1}(-1)^l\frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\|^{2l}}{l!(\sigma_t)^{2l}}\\
&\quad\cdot\sum_{l=0}^{\mathscr{L}_2}(-1)^l\frac{\langle w-m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\rangle^l}{l!(\sigma_t)^{2l}}\\
&\quad\cdot-\frac{(w-m_tG^{\omega_j}|_{\widetilde{x}}(z,x))}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z\Bigg\|_\infty\\
&\lesssim \varepsilon_2^{\alpha_X}\sqrt{\log n}\,\widetilde{\varepsilon}_1^{-d_Y}.
\end{aligned}$$

Furthermore, we can write

$$\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},c_4\varepsilon_1)} \sum_{l=0}^{\mathscr{L}_1}(-1)^l \frac{\|m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\|^{2l}}{l!(\sigma_t)^{2l}}$$
$$\cdot \sum_{l=0}^{\mathscr{L}_2}(-1)^l \frac{\langle w-m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x), m_tG^*_{[k]}|_{\widetilde{x}}(\overline{z}_j,x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\rangle^l}{l!(\sigma_t)^{2l}}$$
$$\cdot -\frac{(w-m_tG^{\omega_j}|_{\widetilde{x}}(z,x))}{\sigma_t}\widetilde{\rho}_j(z)v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z$$
$$=\sum_{l_1=0}^{\mathscr{L}_1}\sum_{l_2=0}^{\mathscr{L}_2}(\frac{1}{\sigma_t})^{2l_1+2l_2+1}\sum_{0\le k\le 2l_1+2l_2+1} m_t^k \sum_{i\in\mathbb{N}_0^{D_Y},|i|\le l_2+1} w^{(i)} \sum_{s\in\mathbb{N}_0^{D_X},|s|\le(2l_1+2l_2+1)\lfloor\beta_X\rfloor+\lfloor\alpha_X\rfloor} a_{l_1l_2kil}\cdot x^{(s)}.$$

So similar to Case 1, let $\mathscr{L}=\mathscr{L}_1\mathscr{L}_2\cdot(2\mathscr{L}_1+2\mathscr{L}_2+1)\binom{\mathscr{L}_2+D_Y}{D_Y}\binom{(2\mathscr{L}_1+2\mathscr{L}_2+1)\lfloor\beta_X\rfloor+\lfloor\alpha_X\rfloor+D_X}{D_X}$, there exists a network $\phi_j^{[1]}(w,x,t)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^4 n)$, $\|W\|_\infty=\Theta\big(\log^6 n\mathscr{L}\big)$, $R=\Theta\big(\log^8 n\mathscr{L}\big)$, $B=\exp(\Theta(\log^4 n))$ so that (10) holds with $\epsilon=\mathcal{O}(\varepsilon_2^{\alpha_X})$. The construction of $\phi_j^{[2]}(w,x,t)$ follows a similar approach. By utilizing the same analysis as in Case 1, we can establish the desired claim 2.

Remark C.2. *Here similar to Case 1, choosing $\delta=0$ will result in a factor of $(\log n)^{D_Y}$ due to the orders of $\mathscr{L}_1$ and $\mathscr{L}_2$ being $\Theta(\log n)$. Instead, we can choose δ as a small positive number so that $\mathscr{L}_1$ and $\mathscr{L}_2$ will be of constant order, and the influence on the neural network size will be $\mathcal{O}(n^{\delta d_Y})$.*

C.1.3 Case 3: $n^{-\frac{2}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}}\le \underline{t}\le c'\,n^{-2\delta}\log^{-3} n$

Set $\varepsilon_1=\sigma_{\underline{t}}\sqrt{\log n}$ and $\varepsilon_2=n^{-\frac{1}{2\alpha_X+d_X}}(\sigma_{\underline{t}}\sqrt{\log n})^{-\frac{d_Y}{2\alpha_X+d_X}}$. Let $\mathcal{N}^X_{\varepsilon_2}$ be one of the largest ε_2-packing of $\mathcal{M}_X$ and $\mathcal{N}^Z_{\varepsilon_1}$ be one of the largest ε_1-packing of $\mathbb{B}_{\mathbb{R}^{d_Y}}(0,\overline{r})$. Then we have $J_1:=|\mathcal{N}^Z_{\varepsilon_1}|\lesssim\varepsilon_1^{-d_Y}$ and $J_2:=|\mathcal{N}^X_{\varepsilon_2}|\lesssim\varepsilon_2^{-d_X}$. Now we take an arbitrary $\widetilde{x}\in\mathcal{N}^X_{\varepsilon_2}$, $k\in\mathcal{K}_{\widetilde{x}}$ and $\widetilde{z}\in N^Z_{\varepsilon_1}$, consider set

$$\mathscr{S}_{k\widetilde{x}\widetilde{z}}=\Big\{(x,w)\;:\;x\in\mathbb{B}_{\mathcal{M}_X}(\widetilde{x},\sqrt{2}\varepsilon_2),$$
$$\|w-G^*_{[k]}(\widetilde{z},x)\|\le C\,\sigma_{\underline{t}}\sqrt{\log n},\mathrm{dist}(w,\mathcal{M}_{Y|x})\le c_0\sigma_{\underline{t}}\sqrt{\log n}\Big\},$$

we claim that

Claim 3. *Let $\mathscr{L}_1=\Theta(\log n)$, $\mathscr{L}_2=\lceil\frac{-2\log n}{\log\sigma_{\underline{t}}+\frac{3}{2}\log(\log n)}\rceil\vee\lceil\frac{-2\log n}{\alpha_Y\log\sigma_{\underline{t}}}\rceil$ and*

$$\mathscr{L}=\mathscr{L}_1\mathscr{L}_2\cdot(2\mathscr{L}_1+2\mathscr{L}_2+1)\binom{(2\mathscr{L}_1+2\mathscr{L}_2+1)\lfloor\beta_Y\rfloor+d_Y}{d_Y}\binom{\mathscr{L}_2+D_Y}{D_Y}\binom{(2\mathscr{L}_1+2\mathscr{L}_2+1)\lfloor\beta_X\rfloor+\lfloor\alpha_X\rfloor+D_X}{D_X}$$

there exists networks $\phi^*(w,x,t)\in\Phi\big(H,W,R,B,\Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ with $H=\Theta(\log^4 n)$, $\|W\|_\infty=\Theta\big(\log^6 n\mathscr{L}\big)$, $R=\Theta\big(\log^8 n\mathscr{L}\big)$, $B=\exp(\Theta(\log^4 n))$, so that for any $(x,w)\in\mathscr{S}_{k\widetilde{x}\widetilde{z}}$, and $t\in[\underline{t},\overline{t}]$,

$$\|\phi^*(w,x,t)-\nabla\log p_{t|x}(w)\|_\infty\lesssim\log n\frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}^2}+\sqrt{\log n}\frac{\varepsilon_2^{\alpha_X}}{\sigma_{\underline{t}}}.$$

Then, similar to Case 1 and 2, by setting $\delta=0$, the second statement of Lemma C.2 directly follows from Lemmas C.4 and C.6. Now we show Claim 3.

For any $(x,w)\in\mathscr{S}_{k\widetilde{x}\widetilde{z}}$, denote $\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)$ as the projection of w to $\mathcal{M}_{Y|x}$, we have

$$\|G^*_{[k]}(\widetilde{z},x)-\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)\|\le\|G^*_{[k]}(\widetilde{z},x)-w\|+\mathrm{dist}(w,\mathcal{M}_{Y|x})\le c_1\sigma_{\underline{t}}\sqrt{\log n}.$$

So

$$
\begin{aligned}
\{y \in \mathcal{M}_{Y|x} : \|y-w\| \le c_2\sigma_{\underline{t}}\sqrt{\log n}\} &\subset \{y \in \mathcal{M}_{Y|x} : \|y - \mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)\| \le c_3\sigma_{\underline{t}}\sqrt{\log n}\} \\
&\subset \{y \in \mathcal{M}_{Y|x} : \|y - G^*_{[k]}(\widetilde{z}, x)\| \le c_4\sigma_{\underline{t}}\sqrt{\log n}\} \\
&\subset \{y = G^*_{[k]}(z, x) : \|z - \widetilde{z}\| \le c_5\sigma_{\underline{t}}\sqrt{\log n}\}.
\end{aligned}
$$

Therefore, by equation (2), we only need to approximate

$$
\frac{1}{\sigma_t} \cdot \frac{\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|w-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot\left(-\frac{w-m_tG^*_{[k]}(z,x)}{\sigma_t}\right) v^*_{[k]}(z|x)\,\mathrm{d}z}{\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|w-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) v^*_{[k]}(z|x)\,\mathrm{d}z}. \tag{11}
$$

Now we consider the polynomial approximation of $G^*_{[k]}$ at $(\widetilde{z}, \widetilde{x})$,

$$
G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z, x) = \sum_{(j_1,j_2)\in\mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}} \frac{G^*_{[k](j_1,j_2)}(\widetilde{z}, \widetilde{x})}{j_1!j_2!}(z-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2}, \tag{12}
$$

we have

$$
\sup_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \; \sup_{x\in\mathbb{B}_{\mathcal{M}_X}(\widetilde{x},\sqrt{2}\varepsilon_2)} \|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z, x) - G^*_{[k]}(z, x)\| \lesssim (\sigma_{\underline{t}}\sqrt{\log n})^{\beta_Y} + \varepsilon_2^{\beta_X}.
$$

Next we present the following lemma, which provides an approximation to the projection function $\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)$.

Lemma C.11. *If $\tau \le \underline{t} \le \log^{-3} n$, then for any fixed $\widetilde{x} \in \mathcal{M}_X$, $k \in \mathcal{K}_{\widetilde{x}}$ and $\widetilde{z} \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$, there exists a neural network $\phi_p(w, x) \in \Phi(H, W, R, B)$ with $H = \Theta(\log^2 n)$, $\|W\|_\infty = \Theta(\log^3 n)$, $R = \Theta(\log^4 n)$ and $B = \exp(\Theta(\log n))$ so that for any $x \in \mathcal{M}_X$ satisfying $\|x - \widetilde{x}\| \lesssim (\sigma_{\underline{t}}\sqrt{\log n})^{\frac{1}{\beta_X}}$, and $w \in \mathbb{R}^{D_Y}$ satisfying $\|w - G^*_{[k]}(\widetilde{z}, x)\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}$ and $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}$, it holds that*

1. $\left\|\left\langle J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(\phi_p(w, x)), w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w, x), x)\right\rangle\right\| \lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y}$.
2. $\left\|\phi_p(w, x) - Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w), x)\right\| \lesssim \sigma_{\underline{t}}\sqrt{\log n}$.

Lemma C.11 suggests that that $G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w, x), x)$ is a good approximation for $\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)$. Based on this, we consider the following decomposition

$$
\begin{aligned}
&\|w - m_tG^*_{[k]}(z, x)\|^2 = \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w, x), x)\|^2 + \|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w, x), x) - m_tG^*_{[k]}(z, x)\|^2 \\
&+ 2\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w, x), x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w, x), x) - m_tG^*_{[k]}(z, x)\rangle.
\end{aligned} \tag{13}
$$

We can then substitute this expression into (11) to obtain

$$\frac{1}{\sigma_t}\cdot\frac{\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|w-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot\left(-\frac{w-m_tG^*_{[k]}(z,x)}{\sigma_t}\right)v^*_{[k]}(z|x)\,\mathrm{d}z}{\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|w-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)v^*_{[k]}(z|x)\,\mathrm{d}z}$$

$$\begin{aligned}
&=\frac{1}{\sigma_t}\cdot\Bigg[\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\Bigg]^{-1}\\
&\quad\cdot\Bigg[\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot\left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)}{\sigma_t}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\Bigg]-\frac{w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)}{\sigma_t^2}
\end{aligned}$$

For the term $-\frac{w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)}{\sigma_t^2}$, since $G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}$ is a polynomial function, using Lemmas C.7-C.10, we can obtain that there exists a neural network $\phi^{[3]}(w,x,t)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^2 n)$, $\|W\|=\Theta(\log^3 n)$, $R=\Theta(\log^4 n)$ and $B=\exp(\Theta(\log^2 n))$ so that

$$\left\|\frac{w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x))}{\sigma_t^2}-\phi^{[3]}(w,x,t)\right\|_\infty\le\frac{1}{n}. \tag{14}$$

Then for the remaining term, notice that for any $(x,w)\in\mathscr{S}_{k\widetilde{x}\widetilde{z}}$ and $\|z-\widetilde{z}\|\lesssim\sigma_{\underline{t}}\sqrt{\log n}$,

$$\|\phi_p(w,x)-\widetilde{z}\|\le\|\phi_p(w,x)-Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),x)\|+\|Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),x)-Q^*_{[k]}(G^*_{[k]}(\widetilde{z},x),x)\|\lesssim\sigma_{\underline{t}}\sqrt{\log n},$$

$$\begin{aligned}
&\left\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\right\|\\
&\le\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\widetilde{z},x)\|+\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\widetilde{z},x)-G^*_{[k]}(\widetilde{z},x)\|\\
&\qquad+\|G^*_{[k]}(\widetilde{z},x)-G^*_{[k]}(z,x)\|+\|(1-m_t)G^*_{[k]}(z,x)\|\\
&\lesssim\|\phi_p(w,x)-\widetilde{z}\|+\varepsilon_2^{\beta_X}+\|z-\widetilde{z}\|+\underline{t}\\
&\lesssim\sigma_{\underline{t}}\sqrt{\log n},\\
&\|w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)\|\le\|w-G^*_{[k]}(\widetilde{z},x)\|+\|G^*_{[k]}(\widetilde{z},x)-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\widetilde{z},x)\|\\
&\qquad+\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\widetilde{z},x)-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)\|\\
&\qquad\lesssim\sigma_{\underline{t}}\sqrt{\log n},
\end{aligned}\tag{15}$$

and

$$\begin{aligned}
&\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle\right|\\
&\le\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle\right|\\
&+\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)-G^*_{[k]}(z,x)\rangle\right|\\
&+\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}(z,x)-m_tG^*_{[k]}(z,x)\rangle\right|\\
&\le\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(\phi_p(w,x))(\phi_p(w,x)-z))\rangle\right|+\mathcal{O}((\sigma_{\underline{t}}\sqrt{\log n})^3)\\
&+\mathcal{O}((\sigma_{\underline{t}}\sqrt{\log n})^{\beta_Y+1})+\mathcal{O}(\sigma_{\underline{t}}\sqrt{\log n}\cdot\varepsilon_2^{\beta_X})\\
&=\mathcal{O}(\sigma_{\underline{t}}^3\log n^{\frac{3}{2}}+\sigma_{\underline{t}}^{\alpha_Y+2}).
\end{aligned}\tag{16}$$

Therefore, denote

$$\overline{dp}_t(w,x) = \int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)$$
$$\cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)$$
$$\cdot \left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)}{\sigma_t}\right) v^*_{[k]}(z|x)\,\mathrm{d}z,$$

and

$$\overline{p}_t(w,x) = \int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)$$
$$\cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) v^*_{[k]}(z|x)\,\mathrm{d}z,$$

we can derive

$$\left\|\frac{\overline{dp}_t(w,x)}{\overline{p}_t(w,x)}\right\| \lesssim \sqrt{\log n},$$

and

$$\overline{p}_t(w,x) \ge \int_{\|z-\phi_p(w,x)\|\le\sigma_{\underline{t}}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)$$
$$\cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) v^*_{[k]}(z|x)\,\mathrm{d}z$$
$$\gtrsim \int_{\|z-\phi_p(w,x)\|\le\sigma_{\underline{t}}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^2}{2\sigma_t^2}\right) v^*_{[k]}(z|x)\,\mathrm{d}z \gtrsim (\sigma_{\underline{t}})^{d_Y}.$$

Therefore, if there exist neural networks $\phi^{[1]}(w,x,t)$ and $\phi^{[2]}(w,x,t)$ so that for any $t\in[\underline{t},\overline{t}]$ and $(x,w)\in\mathscr{S}_{k\widetilde{x}\widetilde{z}}$,

$$\|\overline{dp}_t(w,x) - \phi^{[1]}(w,x,t)\|_\infty = \mathcal{O}\left((\sigma_{\underline{t}})^{d_Y}(\log n\cdot\frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}} + \sqrt{\log n}\cdot\varepsilon_2^{\alpha_X})\right), \tag{17}$$

$$\|\overline{p}_t(w,x) - \phi^{[2]}(w,x,t)\|_\infty = \mathcal{O}\left((\sigma_{\underline{t}})^{d_Y}(\sqrt{\log n}\cdot\frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}} + \varepsilon_2^{\alpha_X})\right). \tag{18}$$

Then we have

$$\left\|\frac{1}{\sigma_t}\cdot\frac{\overline{dp}_t(x)}{\overline{p}_t(x)} - \frac{1}{\sigma_t}\cdot\frac{\phi^{[1]}(x,t)}{\phi^{[2]}(x,t)}\right\|_\infty = \mathcal{O}\left(\log n\frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}^2} + \sqrt{\log n}\frac{\varepsilon_2^{\alpha_X}}{\sigma_{\underline{t}}}\right). \tag{19}$$

To construct $\phi^{[1]}(w,x,t)$, we approximate $\overline{dp}_t(w,x)$ by polynomials. Let

$$G^*_{[k]}|_{\widetilde{x}}(z,x) = \sum_{\substack{j\in\mathbb{N}_0^{d_X}\\|j|<\beta_X}} \frac{G^*_{[k](0,j)}(z,\widetilde{x})}{j!}(x-\widetilde{x})^j,$$

$$v^*_{[k]}|_{\widetilde{x}}(z,x) = \sum_{\substack{j\in\mathbb{N}_0^{d_X}\\ |j|<\alpha_X}} \frac{v^*_{[k](0,j)}(z,\widetilde{x})}{j!}(x-\widetilde{x})^j,$$

we have

$$\|G^*_{[k]}(z,x) - G^*_{[k]}|_{\widetilde{x}}(z,x)\| \lesssim \|x-\widetilde{x}\|^{\beta_X} \lesssim \varepsilon_2^{\beta_X}.$$

and

$$\|v^*_{[k]}(z,x) - v^*_{[k]}|_{\widetilde{x}}(z,x)\| \lesssim \|x-\widetilde{x}\|^{\alpha_X} \lesssim \varepsilon_2^{\alpha_X}.$$

Therefore,

$$\begin{aligned}
&\Big| \|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\|^2 - \|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2 \Big| \\
&\lesssim \sigma_{\underline{t}}\sqrt{\log n}\cdot \varepsilon_2^{\beta_X};
\end{aligned}$$

$$\begin{aligned}
&\Big| \langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\rangle \\
&- \langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle \Big| \\
&\lesssim \sigma_{\underline{t}}\sqrt{\log n}\cdot \varepsilon_2^{\beta_X}, \\
&\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \mathrm{d}z \\
&\lesssim \int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}(\phi_p(w,x),x) - G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \mathrm{d}z \\
&\lesssim \int \exp\left(\frac{-L\|\phi_p(w,x) - z\|^2}{2\sigma_t^2}\right) \mathrm{d}z \\
&\lesssim (\sigma_{\underline{t}})^{d_Y}.
\end{aligned}$$

So we can obtain

$$\begin{aligned}
&\Bigg| \overline{dp}_t(w,x) - \int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\qquad \cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\right) \\
&\qquad \cdot \left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)}{\sigma_t}\right) v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z \Bigg| \\
&\lesssim (\sigma_{\underline{t}})^{d_Y}\cdot\Big(\frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}}\log n + \sqrt{\log n}\cdot\varepsilon_2^{\alpha_X}\Big).
\end{aligned}$$

Similarly,

$$\begin{aligned}
&\Bigg| \overline{p}_t(w,x) - \int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\qquad \cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2}\right) v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z \Bigg| \\
&\lesssim (\sigma_{\underline{t}})^{d_Y}\cdot\Big(\frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}}\sqrt{\log n} + \varepsilon_2^{\alpha_X}\Big).
\end{aligned}$$

Using (15) and (16), by choosing $\mathscr{L}_1 = \Theta(\log n)$ and $\mathscr{L}_2 = \lceil \frac{-2\log n}{\log \sigma_{\underline{t}} + \frac{3}{2}\log(\log n)} \rceil \vee \lceil \frac{-2\log n}{\alpha_Y \log \sigma_{\underline{t}}} \rceil$, we have

$$\begin{aligned}&\Bigg| \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\|^2}{2\sigma_t^2} \right) \\ &- \sum_{l_1=0}^{\mathscr{L}_1} (-1)^{l_1} \frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\|^{2l_1}}{2^{l_1} l_1! \sigma_t^{2l_1}} \Bigg| \lesssim n^{-2},\end{aligned}$$

and

$$\begin{aligned}&\Bigg| \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\rangle}{\sigma_t^2} \right) \\ &- \sum_{l_2=0}^{\mathscr{L}_2} (-1)^{l_2} \frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\rangle^{l_2}}{l_2! \sigma_t^{2l_2}} \Bigg| \\ &\lesssim n^{-2}.\end{aligned}$$

Therefore, we have

$$\begin{aligned}&\Bigg\| \overline{dp}_t(w,x) - \int_{\|z-\widetilde{z}\| \le c_5 \sigma_{\underline{t}} \sqrt{\log n}} \sum_{l_1=0}^{\mathscr{L}_1} (-1)^{l_1} \frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\|^{2l_1}}{2^{l_1} l_1! \sigma_t^{2l_1}} \\ &\quad \cdot \sum_{l_2=0}^{\mathscr{L}_2} (-1)^{l_2} \frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)\rangle^{l_2}}{l_2! \sigma_t^{2l_2}} \\ &\quad \cdot \left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{\widetilde{x}}(z,x)}{\sigma_t} \right) v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z \Bigg\| \\ &\lesssim (\sigma_{\underline{t}})^{d_Y} n^{-1}.\end{aligned} \tag{20}$$

Furthermore, notice that $G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}$, $G^*_{[k]}|_{\widetilde{x}}$ and $v^*_{[k]}|_{\widetilde{x}}$ are both polynomial in x,

$$\begin{aligned}
&\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}} \sum_{l_1=0}^{\mathscr{L}_1}(-1)^{l_1}\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\|^{2l_1}}{2^{l_1}l_1!\sigma_t^{2l_1}} \\
&\quad\cdot\sum_{l_2=0}^{\mathscr{L}_2}(-1)^{l_2}\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)\rangle^{l_2}}{l_2!\sigma_t^{2l_2}} \\
&\quad\cdot\left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{\widetilde{x}}(z,x)}{\sigma_t}\right)v^*_{[k]}|_{\widetilde{x}}(z|x)\,\mathrm{d}z \\
&=\int_{\|z-\widetilde{z}\|\le c_5\sigma_{\underline{t}}\sqrt{\log n}}\sum_{l_1=0}^{\mathscr{L}_1}\sum_{l_2=0}^{\mathscr{L}_2}\frac{(-1)^{(l_1+l_2+1)}}{2^{l_1}l_1!l_2!}(\frac{1}{\sigma_t})^{2l_1+2l_2+1}\Big\|\sum_{(j_1,j_2)\in\mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}}\frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1!j_2!}(\phi_p(w,x)-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2} \\
&\quad-m_t\sum_{\substack{j\in\mathbb{N}_0^{d_X}\\|j|<\beta_X}}\frac{G^*_{[k](0,j)}(z,\widetilde{x})}{j!}(x-\widetilde{x})^j\Big\|^{2l_1}\cdot\Big\langle w-\sum_{(j_1,j_2)\in\mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}}\frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1!j_2!}(\phi_p(w,x)-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2}, \\
&\quad\sum_{(j_1,j_2)\in\mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}}\frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1!j_2!}(\phi_p(w,x)-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2}-m_t\sum_{\substack{j\in\mathbb{N}_0^{d_X}\\|j|<\beta_X}}\frac{G^*_{[k](0,j)}(z,\widetilde{x})}{j!}(x-\widetilde{x})^j\Big\rangle^{l_2} \\
&\cdot\Big(\sum_{(j_1,j_2)\in\mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}}\frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1!j_2!}(\phi_p(w,x)-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2}-m_t\sum_{\substack{j\in\mathbb{N}_0^{d_X}\\|j|<\beta_X}}\frac{G^*_{[k](0,j)}(z,\widetilde{x})}{j!}(x-\widetilde{x})^j\Big) \\
&\quad\cdot\sum_{j_1\in\mathbb{N}_0^{D_X},|j_1|<\alpha_X}\frac{v^*_{[k](0,j_1)}(z|\widetilde{x})}{j_1!}(x-\widetilde{x})^{j_1}\,\mathrm{d}z \\
&=\sum_{l_1=0}^{\mathscr{L}_1}\sum_{l_2=0}^{\mathscr{L}_2}(\frac{1}{\sigma_t})^{2l_1+2l_2+1}\sum_{0\le k\le 2l_1+l_2+1}m_t^k\sum_{s\in\mathbb{N}_0^{d_Y},|s|\le(2l_1+2l_2+1)\lfloor\beta_Y\rfloor}(\phi_p(w,x))^{(s)}\sum_{i\in\mathbb{N}_0^{D_Y},|i|\le l_2}w^{(i)} \\
&\quad\sum_{j\in\mathbb{N}_0^{D_X},|j|\le(2l_1+2l_2+1)\lfloor\beta_X\rfloor+\lfloor\alpha_X\rfloor}a_{l_1l_2ksij}x^{(j)},
\end{aligned}$$

where $a_{l_1l_2ksij}\in\mathbb{R}^{D_Y}$ are some constant coefficients. Then notice that $(\frac{1}{\sigma_t})^{2l_1+2l_2+1}a_{l_1l_2ksij}\lesssim\exp(\mathcal{O}(\log^2 n))$, we

1. Approximate m_t by $\phi_m(t)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^4 n)$, $\|W\|_\infty=\Theta(\log^6 n)$, $R=\Theta(\log^8 n)$ and $B=\exp(\Theta(\log^4 n))$.

2. Approximate σ_t by $\phi_\sigma(t)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^4 n)$, $\|W\|_\infty=\Theta(\log^6 n)$, $R=\Theta(\log^8 n)$ and $B=\exp(\Theta(\log^4 n))$.

3. Approximate $\frac{1}{x}$ by $\phi_{rec}(x)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^4 n)$, $\|W\|_\infty=\Theta(\log^6 n)$, $R=\Theta(\log^8 n)$ and $B=\exp(\Theta(\log^4 n))$.

4. For vector $x\in\mathbb{R}^{D_Y}$, approximate $x^{(i)}$ by $\phi^{[D]}_{vpower}(x;i)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^2 n\cdot\log\log n)$, $\|W\|_\infty=\Theta(\log n)$, $R=\Theta(\log^3 n)$ and $B=\exp(\Theta(\log n\cdot\log\log n)$.

5. For vector $z\in\mathbb{R}^{d_Y}$, approximate $z^{(i)}$ by $\phi^{[d]}_{vpower}(z;i)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^2 n\cdot\log\log n)$, $\|W\|_\infty=\Theta(\log n)$, $R=\Theta(\log^3 n)$ and $B=\exp(\Theta(\log n\cdot\log\log n)$.

6. For $x \in \mathbb{R}$, Approximate x^a by $\phi_{power}(x;a) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n \cdot \log\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log^3 n)$ and $B = \exp(\Theta(\log n \cdot \log\log n))$.

7. For $x, y \in \mathbb{R}$, Approximate $x \cdot y$ by $\phi_{mult}(x,y) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n)$, $\|W\|_\infty = \Theta(1)$, $R = \Theta(\log^2 n)$ and $B = \exp(\Theta(\log^2 n))$.

We have

$$\Bigg\| \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} \Big(\frac{1}{\sigma_t}\Big)^{2l_1+2l_2+1} \sum_{0 \le k \le 2l_1+l_2+1} m_t^k \sum_{s \in \mathbb{N}_0^{d_Y}, |s| \le (2l_1+2l_2+1)\lfloor \beta_Y \rfloor} (\phi_p(w,x))^{(s)} \sum_{i \in \mathbb{N}_0^{D_Y}, |i| \le l_2} w^{(i)} \sum_{j \in \mathbb{N}_0^{D_X}, |j| \le (2l_1+2l_2+1)\lfloor \beta_X \rfloor + \lfloor \alpha_X \rfloor} a_{l_1 l_2 ksij} x^{(j)}$$
$$- \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} \sum_{0 \le k \le 2l_1+l_2+1} \sum_{s \in \mathbb{N}_0^{d_Y}, |s| \le (2l_1+2l_2+1)\lfloor \beta_Y \rfloor} \sum_{i \in \mathbb{N}_0^{D_Y}, |i| \le l_2+1} \sum_{j \in \mathbb{N}_0^{D_X}, |j| \le (2l_1+2l_2+1)\lfloor \beta_X \rfloor + \lfloor \alpha_X \rfloor} a_{l_1 l_2 ksij}$$
$$\cdot \phi_{mult}\Big(\phi_{mult}\Big(\phi_{mult}\Big(\phi_{mult}\Big(\phi_{power}\big(\phi_{rec}(\phi_\sigma(t)); 2l_1+2l_2+1\big), \phi_{power}\big(\phi_m(t); k\big)\Big)$$
$$, \phi_{vpower}^{[d_Y]}(\phi_p(w,x); s)\Big), \phi_{vpower}^{[D_Y]}(\omega; i)\Big), \phi_{vpower}^{[D_X]}(x; j)\Big)\Bigg\|_\infty$$
$$\lesssim (\sigma_{\underline{t}})^{d_Y} n^{-1}.$$

Therefore, by concatenation and parallelization of neural networks, let $\mathscr{L} = \mathscr{L}_1 \mathscr{L}_2 \cdot (2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\binom{(2\mathscr{L}_1+2\mathscr{L}_2+1)\lfloor \beta_Y \rfloor + d_Y}{d_Y}\binom{\mathscr{L}_2 + D_Y}{D_Y}\binom{(2\mathscr{L}_1+2\mathscr{L}_2+1)\lfloor \beta_X \rfloor + \lfloor \alpha_X \rfloor + D_X}{D_X}$, there exists networks $\phi_j^{[1]}(w,x,t) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta\big(\log^6 n \mathscr{L}\big)$, $R = \Theta\big(\log^8 n \mathscr{L}\big)$, $B = \exp(\Theta(\log^4 n))$ so that (17) holds. Similarly, there exists a neural network $\phi^{[2]}(x,t)$ with the same size as $\phi^{[1]}(x,t)$ so that (18) holds. Then using (14), (19), and Lemmas C.7-C.10, we can obtain

$$\Bigg\| \max\Bigg\{ \frac{-c_2\sqrt{\log n}}{\sigma_{\underline{t}}}, \min\Bigg\{ \frac{c_2\sqrt{\log n}}{\sigma_{\underline{t}}}, \phi_{mult}\Big(\phi_{rec}\left(\phi_\sigma(t)\right), \phi_{mult}\Big(\phi^{[1]}(w,x,t), \phi_{rec}(\phi^{[2]}(w,x,t))\Big)\Big)$$
$$- \phi^{[3]}(w,x,t)\Bigg\}\Bigg\} - \nabla \log p_{t|x}(w)\Bigg\|_\infty \lesssim \log n \cdot \frac{\varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}^2} + \sqrt{\log n} \cdot \frac{\varepsilon_2^{\alpha_X}}{\sigma_{\underline{t}}}.$$

We can then obtain Claim 3 by combining all pieces.

Remark C.3. *Here the neural network size has a factor of $(\log n)^{D_X}$ even with the choice of $\delta > 0$. However, we can weaken this factor to $(\log n)^{d_X}$ by assuming that $\mathcal{M}_X$ lies in a smooth d_X-dimensional submanifold. In this case, let $V_{\widetilde{x}} \in \mathbb{R}^{D_X \times d_X}$ be an arbitrary orthonormal basis of the tangent space of $\mathcal{M}_X$ at $\widetilde{x}$, and consider the map $\phi_{\widetilde{x}}(\cdot) = V_{\widetilde{x}}^T(\cdot - \widetilde{x})$. This map is defined on $\mathbb{B}_{\mathcal{M}_X}(\widetilde{x}, r)$ and has a smooth inverse $\phi_{\widetilde{x}}^{-1}$ for some positive r. By expressing x in terms of $\phi_{\widetilde{x}}^{-1}(\phi_{\widetilde{x}}(x))$ and considering the Taylor expansion of $\phi_{\widetilde{x}}^{-1}$ around 0, we can approximate $\overline{p}_t(w,x)$ and $\underline{dp}_t(w,x)$ using polynomials that depend on $\phi_p(w,x)$, w, and $\phi_{\widetilde{x}}(x)$. Notice that $\phi_{\widetilde{x}}(x)$ is d_X-dimensional and can be exactly realized through a ReLU neural network. By leveraging this fact, we can change the factor of $(\log n)^{D_X}$ to $(\log n)^{d_X}$.*

C.1.4 Case 4: $\tau \le \underline{t} \le n^{-\frac{2}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}}$

We set $\varepsilon_1 = n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}}$ and $\varepsilon_2 = n^{-\frac{1}{2\alpha_X + d_X + d_Y \frac{\alpha_X}{\alpha_Y}}}$. Let $\mathcal{N}_{\varepsilon_2}^X$ be one of the largest ε_2-packing of $\mathcal{M}_X$ and $\mathcal{N}_{\varepsilon_1}^Z$ be one of the largest ε_1-packing of $\mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$. Then we have $J_1 := |\mathcal{N}_{\varepsilon_1}^Z| \lesssim \varepsilon_1^{-d_Y}$ and

$J_2 := |\mathcal{N}_{\varepsilon_2}^X| \lesssim \varepsilon_2^{-d_X}$. Then take an arbitrary $\widetilde{x} \in \mathcal{N}_{\varepsilon_2}^X$, $k \in \mathcal{K}_{\widetilde{x}}$ and $\widetilde{z} \in N_{\varepsilon_1}^Z$, Consider set

$$\mathscr{S}_{k\widetilde{x}\widetilde{z}} = \Big\{(x, w) \,:\, x \in \mathbb{B}_{\mathcal{M}_X}(\widetilde{x}, \sqrt{2}\varepsilon_2),$$
$$\|w - G^*_{[k]}(\widetilde{z}, x)\| \le C\,\varepsilon_1, \mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}\Big\},$$

we claim that

Claim 4. *Let* $\mathscr{L}_1 = \Theta(\log n)$, $\mathscr{L}_2 = \lceil \frac{-2\log n}{\log(\sigma_{\underline{t}}) - \frac{3}{2}\log(\log n)} \rceil$ *and*

$$\mathscr{L} = \mathscr{L}_1\mathscr{L}_2 \cdot (2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\binom{(4\mathscr{L}_1 + 3\mathscr{L}_2 + 3)\lfloor\beta_Y\rfloor + 2d_Y + \lfloor\alpha_Y\rfloor}{d_Y}$$
$$\cdot \binom{\mathscr{L}_2 + D_Y}{D_Y}\binom{(2\mathscr{L}_1 + 2\mathscr{L}_2 + 1)\lfloor\beta_X\rfloor + \lfloor\alpha_X\rfloor + D_X}{D_X},$$

there exists a network $\phi^*(w, x, t) \in \Phi\big(H, W, R, B, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ *with* $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta\big(\log^6 n\mathscr{L}\big)$, $R = \Theta\big(\log^8 n\mathscr{L}\big)$, $B = \exp(\Theta(\log^4 n))$, *so that for any* $(x, w) \in \mathscr{S}_{k\widetilde{x}\widetilde{z}}$, *and* $t \in [\underline{t}, \overline{t}]$,

$$\|\phi^*(w, x, t) - \nabla \log p_{t|x}(w)\|_\infty = \mathcal{O}\Big(\log n\frac{\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}^2} + \sqrt{\log n}\frac{\varepsilon_1^{\alpha_Y}}{\sigma_{\underline{t}}}\Big).$$

Then similar as Case 1, 2 and 3, the first statement of Lemma C.2 directly follows from Lemmas C.4 and C.6. Now we show Claim 4. For any $(x, w) \in \mathscr{S}_{k\widetilde{x}\widetilde{z}}$, we have

$$\|G^*_{[k]}(\widetilde{z}, x) - \mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)\| \lesssim \varepsilon_1,$$

and

$$\{y \in \mathcal{M}_{Y|x} \,:\, \|y - w\| \le c_2\sigma_{\underline{t}}\sqrt{\log n}\} \subset \{y \in \mathcal{M}_{Y|x} \,:\, \|y - \mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)\| \le c_3\sigma_{\underline{t}}\sqrt{\log n}\}$$
$$\subset \{y = G^*_{[k]}(z, x) \,:\, \|z - Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w), x)\| \le c_4\sigma_{\underline{t}}\sqrt{\log n}\}.$$

Using Lemma C.11, we have

$$\|z - \phi_p(w, x)\| \le \|z - Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w), x)\| + \|\phi_p(w, x) - Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w), x)\|$$
$$\le \|z - Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w), x)\| + \mathcal{O}\left(\sigma_{\underline{t}}\sqrt{\log n}\right),$$

and thus

$$\{y = G^*_{[k]}(z, x) \,:\, \|z - Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w), x)\| \le c_4\sigma_{\underline{t}}\sqrt{\log n}\}$$
$$\subset \{y = G^*_{[k]}(z, x) \,:\, \|z - \phi_p(w, x)\| \le c_5\sigma_{\underline{t}}\sqrt{\log n}\}$$
$$\subset \{y = G^*_{[k]}(z, x) \,:\, \|z - \phi_p(w, x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}\}.$$

So based on equation (2) and decomposition (13), we only need to approximate

$$
\begin{aligned}
&\frac{1}{\sigma_t}\cdot\frac{\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|w-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot\left(-\frac{w-m_tG^*_{[k]}(z,x)}{\sigma_t}\right)v^*_{[k]}(z|x)\,\mathrm{d}z}{\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|w-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)v^*_{[k]}(z|x)\,\mathrm{d}z}\\
&=\frac{1}{\sigma_t}\cdot\left[\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\right.\\
&\qquad\left.\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\right]^{-1}\\
&\quad\cdot\left[\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\right.\\
&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\left.\cdot\left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)}{\sigma_t}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\right]-\frac{w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)}{\sigma_t^2}
\end{aligned}
\tag{21}
$$

Similar to Case 3, the term $\frac{w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)}{\sigma_t^2}$ can be approximated by neural network $\phi^{[3]}(w,x,t)\in\Phi(H,W,R,B)$ with an error $\frac{1}{n}$ if $H=\Theta(\log^2 n)$, $\|W\|_\infty=\Theta(\log^3 n)$, $R=\Theta(\log^4 n)$ and $B=\exp(\Theta(\log^2 n))$. Then notice that $v^*_{[k]}$ is C^{α_Y,α_X}-smooth, we can write

$$
v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)=\sum_{(j_1,j_2)\in\mathcal{J}^{d_Y,D_X}_{\alpha_Y,\alpha_X}}\frac{v^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1!j_2!}(z-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2},\tag{22}
$$

where

$$
\|v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)-v^*_{[k]}(z,x)\|\lesssim\|z-\widetilde{z}\|^{\alpha_Y}+\|x-\widetilde{x}\|^{\alpha_X}.
$$

We will first build an approximation to the conditional score function by replacing $G^*_{[k]}$ and $v^*_{[k]}$ with their polynomial approximators, that is, $G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}$ defined in (12) and $v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}$ defined in (22). To bound the approximation error, we will consider and bound the following terms using Lemma C.11 for any $(x,w)\in\mathscr{S}_{k\widetilde{x}\widetilde{z}}$, and any $z\in\mathbb{R}^{d_Y}$ satisfying $\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}$:

$$
\begin{aligned}
\|\phi_p(w,x)-\widetilde{z}\|&\le\|\phi_p(w,x)-Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),x)\|+\|Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),x)-\widetilde{z}\|\\
&=\|\phi_p(w,x)-Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),x)\|+\|Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),x)-Q^*_{[k]}(G^*_{[k]}(\widetilde{z},x),x)\|\\
&\lesssim\varepsilon_1;
\end{aligned}
$$

$$
\begin{aligned}
&\left\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\right\|\\
&\le\left\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\right\|+(1-m_t)\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x))\|\lesssim\sigma_{\underline{t}}\sqrt{\log n};
\end{aligned}
$$

$$
\begin{aligned}
&\frac{1}{\sigma_t^2}\cdot\left|\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2-\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^2\right|\\
&\lesssim\frac{\sigma_{\underline{t}}\sqrt{\log n}\left(\varepsilon_1^{\beta_Y}+\varepsilon_2^{\beta_X}\right)}{\sigma_t^2}\asymp\frac{\sqrt{\log n}\left(\varepsilon_1^{\beta_Y}+\varepsilon_2^{\beta_X}\right)}{\sigma_{\underline{t}}};
\end{aligned}
$$

$$
\begin{aligned}
&\|w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)\|\le\|w-\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)\|\\
&+\|G^*_{[k]}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),x),x)-G^*_{[k]}(\phi_p(w,x),x)\|+\|G^*_{[k]}(\phi_p(w,x),x)-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)\|\\
&\lesssim\sigma_{\underline{t}}\sqrt{\log n};
\end{aligned}
$$

$$
\begin{aligned}
&\frac{1}{\sigma_t^2}\cdot\Big|\big\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\big\rangle\\
&\quad-\big\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)\big\rangle\Big|\\
&\lesssim\frac{\sigma_{\underline t}\sqrt{\log n}\big(\varepsilon_1^{\beta_Y}+\varepsilon_2^{\beta_X}\big)}{\sigma_t^2}\asymp\frac{\sqrt{\log n}\big(\varepsilon_1^{\beta_Y}+\varepsilon_2^{\beta_X}\big)}{\sigma_{\underline t}};
\end{aligned}
$$

$$
\begin{aligned}
&\big|\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)\rangle\big|\\
&\le\Big|\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),J_{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\cdot,x)}(\phi_p(w,x))(\phi_p(w,x)-z)\rangle\Big|\\
&+\Big|\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)-J_{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\cdot,x)}(\phi_p(w,x))(\phi_p(w,x)-z)\rangle\Big|\\
&\qquad+\Big|\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),(1-m_t)G^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)\rangle\Big|\\
&\lesssim(\varepsilon_1\sqrt{\log n})^{2\beta_Y}\sigma_{\underline t}\sqrt{\log n}+\sigma_{\underline t}^3(\log n)^{\frac32}+\sigma_{\underline t}^3\sqrt{\log n}\\
&\lesssim\sigma_{\underline t}^3(\log n)^{\frac32};
\end{aligned}\tag{23}
$$

$$
\begin{aligned}
&\left\|\frac{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)}{\sigma_t}\right\|\\
&\lesssim\left\|\frac{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)}{\sigma_t}-\frac{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)}{\sigma_t}\right\|\\
&+\left\|\frac{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)}{\sigma_t}\right\|+\frac{1-m_t}{\sigma_t}\cdot\|G^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)\|\\
&\lesssim\sqrt{\log n}.
\end{aligned}\tag{24}
$$

Combining all the pieces, we can obtain

$$
\begin{aligned}
&\Bigg|\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline t}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot\left(-\frac{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)}{\sigma_t}\right)v^*_{[k]}(z|x)\,\mathrm dz\\
&-\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline t}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)\|^2}{2\sigma_t^2}\right)\\
&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)\rangle}{\sigma_t^2}\right)\\
&\qquad\cdot\left(-\frac{G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}|_{(\widetilde z,\widetilde x)}(z,x)}{\sigma_t}\right)v^*_{[k]}|_{(\widetilde z,\widetilde x)}(z|x)\,\mathrm dz\Bigg|\\
&\quad\lesssim\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline t}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde z,\widetilde x)}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\mathrm dz\\
&\quad\cdot\Big(\frac{\log n\big(\varepsilon_1^{\beta_Y}+\varepsilon_2^{\beta_X}\big)}{\sigma_{\underline t}}+\sqrt{\log n}\cdot\varepsilon_1^{\alpha_Y}\Big).
\end{aligned}\tag{25}
$$

Similarly, we have

$$
\begin{aligned}
&\Big\| \int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\qquad \cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle}{\sigma_t^2}\right) v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z|x)\,\mathrm{d}z \\
&- \int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\qquad \cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) v^*_{[k]}(z|x)\,\mathrm{d}z \Big\| \\
&\lesssim \int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\mathrm{d}z \\
&\quad \cdot \Big(\frac{\sqrt{\log n}\big(\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X}\big)}{\sigma_{\underline{t}}} + \varepsilon_1^{\alpha_Y}\Big).
\end{aligned} \tag{26}
$$

Denote

$$
\begin{aligned}
\widetilde{dp}_t(w,x) = \int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} &\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle}{\sigma_t^2}\right) \\
&\cdot \left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)}{\sigma_t}\right) v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z|x)\,\mathrm{d}z,
\end{aligned}
$$

and

$$
\begin{aligned}
&\widetilde{p}_t(w,x) \\
&= \int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^2}{2\sigma_t^2}\right) \\
&\qquad \cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle}{\sigma_t^2}\right) v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z|x)\,\mathrm{d}z
\end{aligned}
$$

We will show that if there exist neural networks $\phi^{[1]}(w,x,t)$ and $\phi^{[2]}(w,x,t)$ so that for any $t \in [\underline{t}, \overline{t}]$ and for any $(x,w) \in \mathscr{S}_{k\widetilde{x}\widetilde{z}}$,

$$
\|\widetilde{dp}_t(w,x) - \phi^{[1]}(w,x,t)\|_\infty \lesssim (\sigma_{\underline{t}})^{d_Y}\Big(\Big(\frac{\log n\big(\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X}\big)}{\sigma_{\underline{t}}} + \sqrt{\log n}\varepsilon_1^{\alpha_Y}\Big)\Big), \tag{27}
$$

$$
\|\widetilde{p}_t(w,x) - \phi^{[2]}(w,x,t)\|_\infty \lesssim (\sigma_{\underline{t}})^{d_Y}\Big(\Big(\frac{\sqrt{\log n}\big(\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X}\big)}{\sigma_{\underline{t}}} + \varepsilon_1^{\alpha_Y}\Big)\Big), \tag{28}
$$

then it holds that

$$\Bigg\| \frac{1}{\sigma_t} \cdot \Bigg[\int_{\|z-\phi_p(w,x)\|_\infty \le c_6 \sigma_{\underline{t}} \sqrt{\log n}} \exp\left(- \frac{\| G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2} \right) \cdot \exp\left(- \frac{\langle w - G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2} \right) v^*_{[k]}(z|x)\, \mathrm{d}z \Bigg]^{-1} \cdot \Bigg[\int_{\|z-\phi_p(w,x)\|_\infty \le c_6 \sigma_{\underline{t}} \sqrt{\log n}} \exp\left(- \frac{\| G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2} \right) \cdot \exp\left(- \frac{\langle w - G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2} \right) \cdot \left(- \frac{G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)}{\sigma_t} \right) v^*_{[k]}(z|x)\, \mathrm{d}z \Bigg] - \frac{1}{\sigma_t} \cdot \frac{\phi^{[1]}(w,x,t)}{\phi^{[2]}(w,x,t)} \Bigg\|_\infty \lesssim \log n \frac{\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X}}{\sigma_{\underline{t}}^2} + \sqrt{\log n} \frac{\varepsilon_1^{\alpha_Y}}{\sigma_{\underline{t}}}. \tag{29}$$

To show (29), we first bound $\int_{\|z-\phi_p(w,x)\|_\infty \le c_6 \sigma_{\underline{t}} \sqrt{\log n}} \exp\left(- \frac{\| G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2} \right) \mathrm{d}z$. Notice that

$$\begin{aligned} \|\phi_p(w,x) - z\| &= \|Q^*_{[k]}(G^*_{[k]}(\phi_p(w,x),x),x) - Q^*_{[k]}(G^*_{[k]}(z,x),x)\| \\ &\le L\|G^*_{[k]}(\phi_p(w,x),x) - G^*_{[k]}(z,x)\| \\ &\le \|G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\| + (1-m_t)\|G^*_{[k]}(z,x)\| + \mathcal{O}(\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X}) \\ &\le \|G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\| + O(\sigma_{\underline{t}}), \end{aligned}$$

we have

$$\int_{\|z-\phi_p(w,x)\|_\infty \le c_6 \sigma_{\underline{t}} \sqrt{\log n}} \exp\left(- \frac{\| G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2} \right) \mathrm{d}z \lesssim \sigma_{\underline{t}}^{d_Y}.$$

Therefore, combined with (25) and (26), we can get

$$\Bigg\| \int_{\|z-\phi_p(w,x)\|_\infty \le c_6 \sigma_{\underline{t}} \sqrt{\log n}} \exp\left(- \frac{\| G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2} \right) \cdot \exp\left(- \frac{\langle w - G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2} \right) \cdot \left(- \frac{G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)}{\sigma_t} \right) v^*_{[k]}(z|x)\, \mathrm{d}z - \phi^{[1]}(x,t) \Bigg\|_\infty \lesssim (\sigma_{\underline{t}})^{d_Y} \left(\frac{\log n (\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X})}{\sigma_{\underline{t}}} + \sqrt{\log n}\, \varepsilon_1^{\alpha_Y} \right)$$

and

$$\Bigg| \int_{\|z-\phi_p(w,x)\|_\infty \le c_6 \sigma_{\underline{t}} \sqrt{\log n}} \exp\left(- \frac{\| G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2} \right) \cdot \exp\left(- \frac{\langle w - G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\tilde{z},\tilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2} \right) v^*_{[k]}(z|x)\, \mathrm{d}z - \phi^{[2]}(x,t) \Bigg\|_\infty \lesssim (\sigma_{\underline{t}})^{d_Y} \left(\frac{\sqrt{\log n} (\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X})}{\sigma_{\underline{t}}} + \varepsilon_1^{\alpha_Y} \right).$$

Now use the fact that

$$\begin{aligned}&\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|\\&\le\|G^*_{[k]}(\phi_p(w,x),x)-G^*_{[k]}(z,x)\|+(1-m_t)\|G^*_{[k]}(z,x)\|\\&+\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-G^*_{[k]}(z,x)\|\lesssim\|\phi_p(x,w)-z\|+\mathcal{O}(\sigma_{\underline{t}}),\end{aligned}$$

we have

$$\begin{aligned}&\Bigg\|\Bigg[\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\Bigg]^{-1}\\&\quad\cdot\Bigg[\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)\\&\qquad\cdot\left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)}{\sigma_t}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\Bigg]\Bigg\|\\&\quad\lesssim\sqrt{\log n},\end{aligned}$$

and

$$\begin{aligned}&\int_{\|z-\phi_p(w,x)\|_\infty\le c_6\sigma_{\underline{t}}\sqrt{\log n}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\\&\ge\int_{\|z-\phi_p(w,x)\|\le\sigma_{\underline{t}}}\exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\\&\qquad\cdot\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)v^*_{[k]}(z|x)\,\mathrm{d}z\\&\gtrsim\int_{\|z-\phi_p(w,x)\|\le\sigma_{\underline{t}}}\exp\left(-\frac{\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right)\mathrm{d}z.\end{aligned}$$

Moreover, when $\|z-\phi_p(w,x)\|\le\sigma_{\underline{t}}$,

$$\begin{aligned}&\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-m_tG^*_{[k]}(z,x)\rangle\right|\\&\le\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(\phi_p(w,x))(\phi_p(w,x)-z))\rangle\right|\\&+\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)-J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(\phi_p(w,x))(\phi_p(w,x)-z))\rangle\right|\\&\qquad+\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)-G^*_{[k]}(z,x)\rangle\right|\\&\quad+\left|\langle w-G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x),(1-m_t)G^*_{[k]}(z,x)\rangle\right|\\&\lesssim(\varepsilon_1\sqrt{\log n})^{2\beta_Y}\sigma_{\underline{t}}\sqrt{\log n}+\sigma_{\underline{t}}^3(\log n)^{\frac{3}{2}}+\sigma_{\underline{t}}\sqrt{\log n}(\varepsilon_1^{\beta_Y}+\varepsilon_2^{\beta_X})+\sigma_{\underline{t}}^3\sqrt{\log n}\\&\lesssim\sigma_{\underline{t}}^2\end{aligned}$$

Therefore, we have

$$\int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right) \cdot \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}(z,x)\rangle}{\sigma_t^2}\right) v^*_{[k]}(z|x)\,\mathrm{d}z \gtrsim (\sigma_{\underline{t}})^{d_Y}.$$

We can then show (29) by combining all pieces.

Then we construct $\phi^{[1]}(w,x,t)$ by approximating $\widetilde{dp}_t(w,x)$ with polynomials. Based on statements (23) and (24), by choosing $\mathscr{L}_1 = \Theta(\log n)$ and $\mathscr{L}_2 = \lceil \frac{-2\log n}{\log(\sigma_{\underline{t}}) - \frac{3}{2}\log(\log n)} \rceil$, we have

$$\left| \exp\left(-\frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^2}{2\sigma_t^2}\right) - \sum_{l_1=0}^{\mathscr{L}_1} (-1)^{l_1} \frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^{2l_1}}{2^{l_1} l_1! \sigma_t^{2l_1}} \right| \lesssim n^{-2},$$

and

$$\left| \exp\left(-\frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle}{\sigma_t^2}\right) - \sum_{l_2=0}^{\mathscr{L}_2} (-1)^{l_2} \frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle^{l_2}}{l_2! \sigma_t^{2l_2}} \right| \lesssim n^{-2}.$$

Therefore,

$$\Bigg\| \int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \sum_{l_1=0}^{\mathscr{L}_1} (-1)^{l_1} \frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^{2l_1}}{2^{l_1} l_1! \sigma_t^{2l_1}} \cdot \sum_{l_2=0}^{\mathscr{L}_2} (-1)^{l_2} \frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle^{l_2}}{l_2! \sigma_t^{2l_2}} \cdot \left(-\frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)}{\sigma_t}\right) v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z|x)\,\mathrm{d}z - \widetilde{dp}_t(x) \Bigg\|_\infty \lesssim (\sigma_{\underline{t}})^{d_Y} \left(\frac{\log n(\varepsilon_1^{\beta_Y} + \varepsilon_2^{\beta_X})}{\sigma_{\underline{t}}} + \sqrt{\log n}\varepsilon_1^{\alpha_Y} \right).$$

Moreover, since $G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}$ and $v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}$ are polynomials in z and x , we can write

$$\int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \sum_{l_1=0}^{\mathscr{L}_1} (-1)^{l_1} \frac{\|G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\|^{2l_1}}{2^{l_1} l_1! \sigma_t^{2l_1}}$$
$$\cdot \sum_{l_2=0}^{\mathscr{L}_2} (-1)^{l_2} \frac{\langle w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x), G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)\rangle^{l_2}}{l_2! \sigma_t^{2l_2}}$$
$$\cdot \left(- \frac{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x) - m_t G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)}{\sigma_t} \right) v^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z|x)\,\mathrm{d}z$$
$$= \int_{\|z-\phi_p(w,x)\|_\infty \le c_6\sigma_{\underline{t}}\sqrt{\log n}} \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} \frac{(-1)^{(l_1+l_2+1)}}{2^{l_1} l_1! l_2!} (\frac{1}{\sigma_t})^{2l_1+2l_2+1} \Big\| \sum_{(j_1,j_2)\in \mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}} \frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1! j_2!}$$
$$\cdot \Big((\phi_p(w,x)-\widetilde{z})^{j_1} - m_t(z-\widetilde{z})^{j_1} \Big) (x-\widetilde{x})^{j_2} \Big\|^{2l_1} \cdot \Big\langle w - \sum_{(j_1,j_2)\in \mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}} \frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1! j_2!} (\phi_p(w,x)-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2},$$
$$\sum_{(j_1,j_2)\in \mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}} \frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1! j_2!} \Big((\phi_p(w,x)-\widetilde{z})^{j_1} - m_t(z-\widetilde{z})^{j_1} \Big) (x-\widetilde{x})^{j_2} \Big\rangle^{l_2}$$
$$\cdot \sum_{(j_1,j_2)\in \mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}} \frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1! j_2!} \Big((\phi_p(w,x)-\widetilde{z})^{j_1} - m_t(z-\widetilde{z})^{j_1} \Big) (x-\widetilde{x})^{j_2}$$
$$\cdot \sum_{(j_1,j_2)\in \mathcal{J}^{d_Y,D_X}_{\alpha_Y,\alpha_X}} \frac{v^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1! j_2!} (z-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2}\,\mathrm{d}z$$
$$= \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} (\frac{1}{\sigma_t})^{2l_1+2l_2+1} \sum_{0\le k\le 2l_1+l_2+1} m_t^k \sum_{s\in\mathbb{N}_0^{d_Y}, |s|\le (4l_1+3l_2+2)\lfloor\beta_Y\rfloor + d_Y + \lfloor\alpha_Y\rfloor} (\phi_p(w,x))^{(s)} \sum_{i\in\mathbb{N}_0^{D_Y}, |i|\le l_2} w^{(i)}$$
$$\sum_{j\in\mathbb{N}_0^{D_X}, |j|\le (2l_1+2l_2+1)\lfloor\beta_X\rfloor + \lfloor\alpha_X\rfloor} a_{l_1 l_2 ksij} x^{(j)},$$

where $a_{l_1 l_2 ksij} \in \mathbb{R}^{D_Y}$ are some constant coefficients. Then notice that $(\frac{1}{\sigma})^{2l_1+2l_2+1} a_{l_1 l_2 ksij} \lesssim \exp(\mathcal{O}(\log^2 n))$, we

1. Approximate m_t by $\phi_m(t) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta(\log^6 n)$, $R = \Theta(\log^8 n)$ and $B = \exp(\Theta(\log^4 n))$.

2. Approximate σ_t by $\phi_\sigma(t) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta(\log^6 n)$, $R = \Theta(\log^8 n)$ and $B = \exp(\Theta(\log^4 n))$.

3. Approximate $\frac{1}{x}$ by $\phi_{rec}(x) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \Theta(\log^6 n)$, $R = \Theta(\log^8 n)$ and $B = \exp(\Theta(\log^4 n))$.

4. For vector $x \in \mathbb{R}^{D_Y}$, approximate $x^{(i)}$ by $\phi^{[D]}_{vpower}(x;i) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n)$, $\|W\|_\infty = \Theta(1)$, $R = \Theta(\log^2 n)$ and $B = \exp(\Theta(\log\log n))$.

5. For vector $z \in \mathbb{R}^{d_Y}$, approximate $z^{(i)}$ by $\phi^{[d]}_{vpower}(z;i) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n \cdot \log\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log^3 n)$ and $B = \exp(\Theta(\log n \cdot \log\log n))$.

6. For $x \in \mathbb{R}$, Approximate x^a by $\phi_{power}(x;a) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n \log\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log^3 n)$ and $B = \exp(\Theta(\log n \log\log n)$.

7. For $x, y \in \mathbb{R}$, Approximate $x \cdot y$ by $\phi_{mult}(x,y) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n)$, $\|W\|_\infty = \Theta(1)$, $R = \Theta(\log^2 n)$ and $B = \exp(\Theta(\log^2 n))$.

We have

$$\Bigg\| \sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} \Big(\frac{1}{\sigma_t}\Big)^{2l_1+2l_2+1} \sum_{0\le k\le 2l_1+l_2+1} m_t^k \sum_{s\in\mathbb{N}_0^{d_Y}, |s|\le(4l_1+3l_2+2)\lfloor\beta_Y\rfloor+d_Y+\lfloor\alpha_Y\rfloor} (\phi_p(w,x))^{(s)} \sum_{i\in\mathbb{N}_0^{D_Y}, |i|\le l_2} w^{(i)}$$

$$\sum_{j\in\mathbb{N}_0^{D_X}, |j|\le(2l_1+2l_2+1)\lfloor\beta_X\rfloor+\lfloor\alpha_X\rfloor} a_{l_1l_2ksij} x^{(j)}$$

$$-\sum_{l_1=0}^{\mathscr{L}_1} \sum_{l_2=0}^{\mathscr{L}_2} \sum_{0\le k\le 2l_1+2l_2+1} \sum_{s\in\mathbb{N}_0^{d_Y}, |s|\le(4l_1+3l_2+2)\lfloor\beta_Y\rfloor+d_Y+\lfloor\alpha_Y\rfloor} \sum_{i\in\mathbb{N}_0^{D_Y}, |i|\le l_2+1} \sum_{j\in\mathbb{N}_0^{D_X}, |j|\le(2l_1+2l_2+1)\lfloor\beta_X\rfloor+\lfloor\alpha_X\rfloor} a_{l_1l_2ksij}$$

$$\cdot\,\phi_{mult}\Big(\phi_{mult}\Big(\phi_{mult}\Big(\phi_{mult}\Big(\phi_{power}\big(\phi_{rec}(\phi_\sigma(t)); 2l_1+2l_2+1\big), \phi_{power}\big(\phi_m(t); k\big)\Big)$$

$$, \phi_{vpower}^{[d_Y]}(\phi_p(w,x); s)\Big), \phi_{vpower}^{[D_Y]}(\omega; i)\Big), \phi_{vpower}^{[D_X]}(x; j)\Big)\Bigg\|_\infty$$

$$\lesssim (\sigma_{\underline{t}})^{d_Y}\Big(\frac{\log n\big(\varepsilon_1^{\beta_Y}+\varepsilon_2^{\beta_X}\big)}{\sigma_{\underline{t}}} + \sqrt{\log n}\,\varepsilon_1^{\alpha_Y}\Big).$$

Therefore, let $\mathscr{L} = \mathscr{L}_1\mathscr{L}_2\cdot(2\mathscr{L}_1+2\mathscr{L}_2+1)\binom{(4\mathscr{L}_1+3\mathscr{L}_2+3)\lfloor\beta_Y\rfloor+2d_Y+\lfloor\alpha_Y\rfloor}{d_Y}\binom{\mathscr{L}_2+D_Y}{D_Y}\binom{(2\mathscr{L}_1+2\mathscr{L}_2+1)\lfloor\beta_X\rfloor+\lfloor\alpha_X\rfloor+D_X}{D_X}$, there exists network $\phi^{[1]}(w,x,t)\in\Phi(H,W,R,B)$ with $H=\Theta(\log^4 n)$, $\|W\|_\infty=\Theta\big(\log^6 n\mathscr{L}\big)$, $R=\Theta\big(\log^8 n\mathscr{L}\big)$, $B=\exp(\Theta(\log^4 n))$ so that (27) holds. By employing same techniques, we can also obtain that there exists a neural network $\phi_j^{[2]}(w,x,t)$ with the same size as $\phi_j^{[1]}(x,t)$ so that (28) holds. Then use (29), similar as the analysis for Case 3, we can obtain Claim 4.

C.2 Proof of Lemma C.3

Firstly we have the following lemma whose proof follows [5].

Lemma C.12. *The following equality holds for all $S(w_t,x,t)$ and $t>0$,*

$$\begin{aligned}
&\mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_ty,\sigma_t^2I_{D_Y})}\left[\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\right]\\
&=\mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_ty,\sigma_t^2I_{D_Y})}\left[\|S(w_t,x,t)-\frac{m_tY-w_t}{\sigma_t^2}\|^2\right]\\
&\quad+\mathbb{E}_{\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_ty,\sigma_t^2I_{D_Y})}\left[\left\|\nabla\log p_{t|x}(w_t)\right\|^2-\left\|\frac{m_tY-w_t}{\sigma_t^2}\right\|^2\right].
\end{aligned}$$

Then for any $i\in[\mathcal{I}]$, we denote

$$\ell_i(x,y,S)=\int_{t_{i-1}}^{t_i}\mathbb{E}_{w_t\sim\mathcal{N}(m_ty,\sigma_t^2I_{D_Y})}\left[\|S(w_t,x,t)-\frac{m_ty-w_t}{\sigma_t^2}\|^2\right]\,\mathrm{d}t,$$

and $\rho_i=\sup_{(x,y)\in\mathcal{M}}\sup_{S\in\mathcal{S}_i}|\ell_i(x,y,S)|$, we have

$$\begin{aligned}
&\mathbb{E}_{\mu^*}[\ell_i(x,y,S)]\\
&=\int_{t_{i-1}}^{t_i}\mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_tY,\sigma_t^2I_{D_Y})}\left[\|S(w_t,x,t)-\frac{m_tY-w_t}{\sigma_t^2}\|^2\right]\,\mathrm{d}t\\
&=\int_{t_{i-1}}^{t_i}\mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_ty,\sigma_t^2I_{D_Y})}\left[\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\right]\,\mathrm{d}t\\
&-\int_{t_{i-1}}^{t_i}\mathbb{E}_{\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_ty,\sigma_t^2I_{D_Y})}\left[\left\|\nabla\log p_{t|x}(w_t)\right\|^2-\left\|\frac{m_tY-w_t}{\sigma_t^2}\right\|^2\right]\,\mathrm{d}t,
\end{aligned}$$

and

$$\begin{aligned}\rho_i &\le \sup_{(x,y)\in\mathcal{M}} \sup_{S\in\mathcal{S}_i} \int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})} \left[2\|S(w_t,x,t)\|^2 + 2\|\frac{m_t y - w_t}{\sigma_t^2}\|^2\right] \mathrm{d}t \\ &\lesssim (t_i - t_{i-1}) \cdot \frac{\log n}{t_{i-1}\wedge 1} \\ &\lesssim (\log n)^2.\end{aligned}$$

Let

$$S_i^* \in \arg\min_{S\in\mathcal{S}_i} \mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}[\ell_i(x,y,S)].$$

Consider the function class

$$\overline{G}_i^* = \{g(x,y) = a(\ell_i(x,y,S) - \ell_i(x,y,S_i^*)) \,:\, a\in[0,1], S\in\mathcal{S}_i\},$$

and

$$G_i^* = \{g(x,y) = \ell_i(x,y,S) - \ell_i(x,y,S_i^*) \,:\, S\in\mathcal{S}_i\}.$$

Denote $\|g\|_2 = \sqrt{\mathbb{E}_{\mu^*}[g^2]}$, using standard symmetrization, we can get for any $r > 0$,

$$\mathcal{R}_n(\overline{G}_i^*, r) = \mathbb{E}_{\mu^{*\otimes n}}\left[\sup_{\substack{g\in\overline{G}_i^*\\ \|g\|_2\le r}} \left|\frac{1}{n}\sum_{i=1}^n g(X_i,Y_i) - \mathbb{E}_{\mu^*}\left[g(x,y)\right]\right|\right] \le \mathbb{E}_{\mu^{*\otimes n}}\mathbb{E}_\epsilon\left[\sup_{\substack{g\in\overline{G}^*\\ \|g\|_2\le r}} \left|\frac{2}{n}\sum_{i=1}^n \epsilon_i g(X_i,Y_i)\right|\right],$$

where $\{\epsilon_i\}_{i=1}^n$ are n i.i.d. copies from Rademacher distribution, i.e. $\mathbb{P}(\epsilon_i = 1) = \mathbb{P}(\epsilon_i = -1) = \frac{1}{2}$.

Define $d_n(g,g') = \sqrt{\frac{1}{n}\sum_{i=1}^n (g(X_i,Y_i) - g'(X_i,Y_i))^2}$, then

$$r_{ni} = \max_{\substack{g,g'\in\overline{G}_i^*\\ \|g\|_2,\|g'\|_2\le r}} d_n(g,g') \le 2\rho_i.$$

By equation (3.84) of [6], there exists a constant c such that,

$$\begin{aligned}\mathbb{E}_{\mu^{*\otimes n}}[r_{ni}^2] &\le \mathbb{E}_{\mu^{*\otimes n}}\left[\sup_{\substack{g\in\overline{G}_i^*\\ \|g\|_2\le r}} \frac{4}{n}\sum_{i=1}^n g^2(X_i,Y_i)\right] \\ &\le \mathbb{E}_{\mu^{*\otimes n}}\left[\sup_{\substack{g\in\overline{G}_i^*\\ \|g\|_2\le r}} \frac{8}{n}\sum_{i=1}^n \left(g(X_i,Y_i) - \mathbb{E}_{\mu^*}[g(x,y)]\right)^2\right] + 8r^2 \\ &\le c(r^2 + \rho_i \overline{R}_n(r,\overline{G}_i^*)).\end{aligned}$$

Then for any $g\in G_i^*$ and $a\in(0,1]$, there exists an integer $\kappa\in\mathbb{N}$, such that $\kappa\frac{\varepsilon}{2\rho_i} < a \le (\kappa+1)\frac{\varepsilon}{2\rho_i}$ and $d_n((\kappa+1)\frac{\varepsilon}{2\rho_i} g, ag) \le \frac{\varepsilon}{2\rho_i}\rho_i = \frac{\varepsilon}{2}$. Therefore it follows that the ε-covering number of $\overline{G}_i^*$ satisfies that,

$\mathbf{N}(\overline{G}_i^*, d_n, \varepsilon) \leq \mathbf{N}(G_i^*, d_n, \frac{\varepsilon}{2})\frac{2\rho_i}{\varepsilon}$ and $\log \mathbf{N}(\overline{G}_i^*, d_n, \varepsilon) \leq \log \mathbf{N}(G_i^*, d_n, \frac{\varepsilon}{2}) + \log \frac{2\rho_i}{\varepsilon}$. Moreover,

$$\forall g = \ell(x, y, S) - \ell(x, y, S_i^*), g' = \ell(x, y, S') - \ell(x, y, S_i^*) \in G_i^*,$$

$$
\begin{aligned}
&d_n(g, g') \\
&= \sqrt{\frac{1}{n}\sum_{i=1}^n \Big(\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_tY_i,\sigma_t^2 I_{D_Y})}\left[\|S(w_t, X_i, t) - \frac{m_tY_i - w_t}{\sigma_t^2}\|^2 - \|S'(w_t, X_i, t) - \frac{m_tY_i - w_t}{\sigma_t^2}\|^2\right] \mathrm{d}t\Big)^2} \\
&\leq \Big(\frac{1}{n}\sum_{i=1}^n \int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_tY_i,\sigma_t^2 I_{D_Y})}\|S(w_t, X_i, t) - S'(w_t, X_i, t)\|^2 \,\mathrm{d}t \\
&\quad\cdot \int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_tY_i,\sigma_t^2 I_{D_Y})}\|S(w_t, X_i, t) + S'(w_t, X_i, t) - 2\frac{m_tY_i - w_t}{\sigma_t^2}\|^2 \,\mathrm{d}t\Big)^{\frac{1}{2}} \\
&\lesssim \log n \cdot \Big(\frac{1}{n}\sum_{i=1}^n \int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_tY_i,\sigma_t^2 I_{D_Y})}\|S(w_t, X_i, t) - S'(w_t, X_i, t)\|^2 \,\mathrm{d}t\Big)^{\frac{1}{2}} \\
&\lesssim (\log n)^{\frac{3}{2}} \sup_{\substack{x\in\mathcal{M}_X, w\in[-c\sqrt{\log n}, c\sqrt{\log n}]^{D_Y} \\ t\in[t_{i-1}, t_i]}} \|S(w, x, t) - S'(w, x, t)\| + \frac{1}{n^2}.
\end{aligned}
$$

By standard result for covering number of neural network (e.g., Lemma 3 of [3]), we have for any $\varepsilon \geq \frac{1}{n^2}$

$$\log \mathbf{N}(G_i^*, d_n, \varepsilon) \lesssim S_i H_i \log\left(\varepsilon^{-1} H_i \|W_i\|_\infty (B_i \vee 1) n\right)$$

Then by Dudley entropy integral bound, we have

$$
\begin{aligned}
&\overline{R}_n(r, \overline{G}_i^*) \lesssim \frac{1}{n^2} + \frac{1}{\sqrt{n}}\mathbb{E}_{\mu^{*\otimes n}}\left[\int_{\frac{1}{n^2}}^{r_{ni}} \sqrt{R_i H_i \log\left(\varepsilon^{-1} H_i \|W_i\|_\infty (B_i \vee 1) n\right)}\,\mathrm{d}\varepsilon\right] \\
&\leq \frac{1}{n^2} + \frac{1}{\sqrt{n}}\mathbb{E}_{\mu^{*\otimes n}}\left[r_{ni}\int_0^1 \sqrt{R_i H_i \log\left(\varepsilon^{-1}\frac{R_i H_i \|W_i\|_\infty (B_i \vee 1) n}{r_{ni}}\right)}\,\mathrm{d}\varepsilon\right] \\
&\lesssim \sqrt{\frac{R_i H_i \log\left(H_i \|W_i\|_\infty (B_i \vee 1) n\right)}{n}}\mathbb{E}_{\mu^{*\otimes n}}[r_{ni}] + \sqrt{\frac{R_i H_i}{n}}\mathbb{E}_{\mu^{*\otimes n}}\left[r_{ni}\sqrt{\log\frac{2\rho_i}{r_{ni}} + \frac{1}{2}}\right] \\
&\lesssim \sqrt{\frac{R_i H_i}{n}}\sqrt{-\frac{1}{2}\mathbb{E}_{\mu^{*\otimes n}}\left[r_{ni}^2 \log \mathbb{E}_{\mu^{*\otimes n}}\left(\frac{r_{ni}}{2\rho_i}\right)^2\right] + \frac{1}{2}\mathbb{E}_{\mu^{*\otimes n}}[r_{ni}^2] + \log\left(H_i \|W_i\|_\infty (B_i \vee 1) n\right)\mathbb{E}_{\mu^{*\otimes n}}[r_{ni}^2]},
\end{aligned}
$$

where the last inequality uses that $\sqrt{-\frac{1}{2}y\log y + \frac{1}{2}y}$ is concave and non-decreasing when $y = (\frac{r_{ni}}{2\rho_i})^2 \leq 1$. Then by $\mathbb{E}_{\mu^{*\otimes n}}[r_{ni}^2] \leq c(r^2 + \rho_i \overline{R}_n(r, \overline{G}^*))$, we have

$$
\begin{aligned}
\overline{R}_n(r, \overline{G}^*) &\lesssim \sqrt{\frac{R_i H_i}{n}}(r^2 + \rho_i \overline{R}_n(r, \overline{G}^*))^{\frac{1}{2}}\sqrt{\log\frac{\rho_i}{r} + \log\left(H_i \|W_i\|_\infty (B_i \vee 1) n\right)} \\
&\lesssim \sqrt{\frac{R_i H_i}{n}}(r^2 + (\log n)^2 \overline{R}_n(r, \overline{G}^*))^{\frac{1}{2}}\sqrt{\log\frac{(\log n)^2}{r} + \log\left(H_i \|W_i\|_\infty (B_i \vee 1) n\right)}
\end{aligned}
$$

Choose $\delta_{ni} = c_2(\log n)^2\frac{\sqrt{R_i H_i \log(R_i H_i \|W_i\|_\infty (B_i \vee 1) n)}}{\sqrt{n}}$, if $\overline{R}_n(\delta_{ni}, \overline{G}^*) > \delta_{ni}^2/(\log n)^2$, then

$$\overline{R}_n(\delta_{ni}, \overline{G}^*) \lesssim \frac{1}{\sqrt{n}}\log n \cdot \overline{R}_n(\delta_{ni}, \overline{G}^*)^{\frac{1}{2}}\sqrt{R_i H_i \log\left(R_i H_i \|W_i\|_\infty (B_i \vee 1) n\right)}$$

which means

$$\overline{R}_n(\delta_{ni}, \overline{G}^*) \lesssim \frac{(\log n)^2}{n} R_i H_i \log\left(R_i H_i \|W_i\|_\infty (B_i \vee 1) n\right) \lesssim \frac{\delta_{ni}^2}{(\log n)^2}.$$

Therefore for a large enough c_2, we have $\overline{R}_n(\delta_{ni}, \overline{G}^*) \le \delta_{ni}^2/(\log n)^2$. Then denote

$$M_{ni}(S) = \frac{1}{n}\sum_{i=1}^{n} \ell_i(X_i, Y_i, S)$$

and

$$M_i^*(S) = \mathbb{E}_{\mu^*}[\ell_i(X, Y, S)],$$

we have the following lemma,

Lemma C.13. *There exist some constants* (c_0, c_1, c_2) *such that it holds with probability larger than* $1 - \frac{1}{n^2}$ *that,*

$\forall S \in \mathcal{S}_i$,

$$\begin{aligned}&\frac{|M_{ni}(S) - M_{ni}(S_i^*) - M_i^*(S) + M_i^*(S_i^*)|}{\delta_{ni} + \|\ell_i(x, y, S) - \ell_i(x, y, S_i^*)\|_2}\\ &\le c_2\delta_{ni}/(\log n)^2.\end{aligned}$$

Therefore, we have

$$\begin{aligned}
&\|\ell_i(x, y, S) - \ell_i(x, y, S_i^*)\|_2^2\\
&= \mathbb{E}_{\mu^*}[(\ell_i(x, y, S) - \ell_i(x, y, S_i^*))^2]\\
&= \mathbb{E}_{\mu^*}\Big[\Big(\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y, \sigma_t^2 I_{D_Y})}\Big[\|S(w_t, x, t) - \frac{m_t y - w_t}{\sigma_t^2}\|^2 - \|S_i^*(w_t, x, t) - \frac{m_t y - w_t}{\sigma_t^2}\|^2\Big]\,\mathrm{d}t\Big)^2\Big]\\
&\le \mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y, \sigma_t^2 I_{D_Y})}\|S(w_t, x, t) - S_i^*(w_t, x, t)\|^2\,\mathrm{d}t\\
&\qquad \cdot \int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y, \sigma_t^2 I_{D_Y})}\|S(w_t, x, t) + S_i^*(w_t, x, t) - 2\frac{m_t y - w_t}{\sigma_t^2}\|^2\,\mathrm{d}t\Big]\\
&\lesssim (\log n)^2 \cdot \mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y, \sigma_t^2 I_{D_Y})}\|S(w_t, x, t) - S_i^*(w_t, x, t)\|^2\,\mathrm{d}t\Big]\\
&\lesssim (\log n)^2 \cdot \mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y, \sigma_t^2 I_{D_Y})}\|S(w_t, x, t) - \nabla \log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]\\
&+ (\log n)^2 \cdot \min_{S\in\mathcal{S}_i}\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y, \sigma_t^2 I_{D_Y})}\|S(w_t, x, t) - \nabla \log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big].
\end{aligned}$$

Then notice that

$$
\begin{aligned}
&\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|\widehat{S}(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]\\
&\qquad-\min_{S\in\mathcal{S}_i}\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]\\
&=\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|\widehat{S}(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]\\
&\qquad-\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|S_i^*(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]\\
&=M_i^*(\widehat{S})-M^*(S_i^*)\\
&\le M_i^*(\widehat{S})-M^*(S_i^*)+M_{ni}(S_i^*)-M_{ni}(\widehat{S})\\
&\le c_2\frac{\delta_{ni}^2}{(\log n)^2}+\frac{\delta_{ni}}{\log n}\cdot\Big(\sqrt{\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|\widehat{S}(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]}\\
&+\sqrt{\min_{S\in\mathcal{S}_i}\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]}\Big)
\end{aligned}
$$

So it holds with probability larger than $1-\frac{1}{n}$ that,

$$
\begin{aligned}
&\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|\widehat{S}(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]\\
&\lesssim\frac{\delta_{ni}^2}{(\log n)^2}+\min_{S\in\mathcal{S}_i}\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big]\\
&\lesssim(\log n)^2\frac{R_iH_i\log\left(R_iH_i\|W_i\|_\infty(B_i\vee 1)n\right)}{n}\\
&\qquad+\min_{S\in\mathcal{S}_i}\mathbb{E}_{\mu^*}\Big[\int_{t_{i-1}}^{t_i} \mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\,\mathrm{d}t\Big].
\end{aligned}
$$

C.3 Proof of Technical Results

C.3.1 Proof of Lemma B.2

For the first statement, denote $\mathrm{vol}_{\mathcal{M}_{Y|x}}$ as the volume measure of $\mathcal{M}_{Y|x}$. Then notice that

$$
\begin{aligned}
&\mathbb{E}_{y\sim\mu^*_{Y|x}}[g(y)\cdot\mathbf{1}(y\in\mathbb{B}_{\mathcal{M}_{Y|x}}(y^*,r))]=\int g(y)\cdot\mathbf{1}(y\in\mathbb{B}_{\mathcal{M}_{Y|x}}(y^*,r))f(y|x)\,\mathrm{dvol}_{\mathcal{M}_{Y|x}}(y)\\
&=\int_{U_{Y|x}^{(x^*,y^*)}} g(y)\cdot\mathbf{1}(y\in\mathbb{B}_{\mathcal{M}_{Y|x}}(y^*,r))f(y|x)\,\mathrm{dvol}_{\mathcal{M}_{Y|x}}(y)\\
&=\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} g(G^*(z,x))\mathbf{1}(y\in\mathbb{B}_{\mathcal{M}_{Y|x}}(y^*,r))f(G^*(z,x)|x)\sqrt{\det(J_{G^*(\cdot,x)}(z)^TJ_{G^*(\cdot,x)}(z))}\,\mathrm{d}z\\
&=\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} g(G^*(z,x))\mathbf{1}(G^*(z,x)\in\mathbb{B}_{\mathcal{M}_{Y|x}}(y^*,r)))v^*(z|x)\,\mathrm{d}z.
\end{aligned}
$$

For the second statement, since $\widetilde{r}\ge r$ and $\{(x_k^*,y_k^*)\}_{k=1}^K\subset\mathcal{M}$ is a $\frac{r}{2}$-cover of $\mathcal{M}$, for any $(x,y)\in\mathcal{M}$, there exists $k'\in[K]$ so that $\|(x_{k'}^*,y_{k'}^*)-(x,y)\|\le\frac{r}{2}\le\frac{\widetilde{r}}{2}$. Therefore, $\sum_{k=1}^K\rho_k(x,y)\ge\rho_{k'}(x,y)=1$

and $\sum_{k=1}^K \widetilde{\rho}_k(x,y) = 1$. So based on $\widetilde{r} \le r_0$ and the first statement, we have

$$\begin{aligned}
\mathbb{E}_{y\sim\mu^*_{Y|x}}[g(y)] &= \sum_{k=1}^K \mathbb{E}_{y\sim\mu^*_{Y|x}}[g(y)\widetilde{\rho}_k(x,y)] \\
&= \sum_{k=1}^K \mathbb{E}_{y\sim\mu^*_{Y|x}}[g(y)\widetilde{\rho}_k(x,y)\cdot \mathbf{1}(y\in \mathbb{B}_{\mathcal{M}_{Y|x}}(y_k,\widetilde{r}))] \\
&= \sum_{k=1}^K \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} g(G^*_{[k]}(z,x))\widetilde{\rho}_k(x,G^*_{[k]}(z,x))\mathbf{1}(G^*_{[k]}(z,x)\in \mathbb{B}_{\mathcal{M}_{Y|x}}(y_k,\widetilde{r}))v^*_{[k]}(z|x)\,\mathrm{d}z \\
&= \sum_{k=1}^K \int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} g(G^*_{[k]}(z,x))\widetilde{\rho}_k(x,G^*_{[k]}(z,x))v^*_{[k]}(z|x)\,\mathrm{d}z.
\end{aligned}$$

C.4 Proof of Lemma C.4

Without loss of generality, we assume for any $x\in\mathcal{M}_X$, $\mathcal{M}_{Y|x}\subset \mathbb{B}_{\mathbb{R}^{D_Y}}(0,1)$. Then for any $w\in\mathbb{R}^{D_Y}$,

$$\begin{aligned}
&\left\|\nabla \log p_{t|x}(w)\right\| = \left\|\frac{\nabla p_{t|x}(w)}{p_{t|x}(w)}\right\| = \left\|\frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w-m_t y)}{\sigma_t^2}\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\right]}\right\| \\
&\le \sqrt{\sum_{l=1}^{D_Y}\left(\frac{|w_l|+1}{\sigma_t^2}\right)^2} \le \frac{\|w\|+\sqrt{D_Y}}{\sigma_t^2}.
\end{aligned}$$

Furthermore, by Lemma B.2, it holds with a large enough constant c that

$$\begin{aligned}
&\int_{\mathbb{R}^{D_Y}} \left\|\nabla \log p_{t|x}(w)\right\|^2 p_{t|x}(w)\mathbf{1}\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\ge c_0\sigma_{t_{i-1}}\sqrt{\log n}\right)\mathrm{d}w \\
&\le \int_{\mathbb{R}^{D_Y}} \frac{\|w\|+\sqrt{D_Y}}{\sigma_t^2}\cdot \mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\frac{1}{(2\pi\sigma_t^2)^{\frac{D_Y}{2}}}\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\right]\mathbf{1}\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\ge c_0\sigma_{t_{i-1}}\sqrt{\log n}\right)\mathrm{d}w \\
&= \sum_{k=1}^K \int_{\mathbb{R}^{D_Y}}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} \frac{\|w\|+\sqrt{D_Y}}{\sigma_t^2}\frac{1}{(2\pi\sigma_t^2)^{\frac{D_Y}{2}}}\cdot\mathbf{1}\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\ge c_0\sigma_{t_{i-1}}\sqrt{\log n}\right) \\
&\quad\cdot\exp\left(-\frac{\|w-m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot \widetilde{\rho}_k(x,G^*_{[k]}(z,x))v^*_{[k]}(z|x)\,\mathrm{d}z\,\mathrm{d}w \\
&\le \sum_{k=1}^K \int_{\mathbb{R}^{D_Y}}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} \frac{\|w\|+\sqrt{D_Y}}{\sigma_t^2}\frac{1}{(2\pi\sigma_t^2)^{\frac{D_Y}{2}}}\cdot\mathbf{1}\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\ge c_0\sigma_{t_{i-1}}\sqrt{\log n}, \|w\|\le c\sqrt{\log n}\right) \\
&\quad\cdot\exp\left(-\frac{\|w-m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot \widetilde{\rho}_k(x,G^*_{[k]}(z,x))v^*_{[k]}(z|x)\,\mathrm{d}z\,\mathrm{d}w \\
&\quad+\sum_{k=1}^K \int_{\mathbb{R}^{D_Y}}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} \frac{\|w\|+\sqrt{D_Y}}{\sigma_t^2}\frac{1}{(2\pi\sigma_t^2)^{\frac{D_Y}{2}}}\cdot\mathbf{1}\left(\|w\|> c\sqrt{\log n}\right) \\
&\quad\cdot\exp\left(-\frac{\|w-m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot \widetilde{\rho}_k(x,G^*_{[k]}(z,x))v^*_{[k]}(z|x)\,\mathrm{d}z\,\mathrm{d}w \\
&\le \sum_{k=1}^K \int_{\mathbb{R}^{D_Y}}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)} \frac{\|w\|+\sqrt{D_Y}}{\sigma_t^2}\frac{1}{(2\pi\sigma_t^2)^{\frac{D_Y}{2}}}\cdot\mathbf{1}\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\ge c_0\sigma_{t_{i-1}}\sqrt{\log n}, \|w\|\le c\sqrt{\log n}\right) \\
&\quad\cdot\exp\left(-\frac{\|w-m_t G^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot \widetilde{\rho}_k(x,G^*_{[k]}(z,x))v^*_{[k]}(z|x)\,\mathrm{d}z\,\mathrm{d}w + \frac{1}{n^2}.
\end{aligned}$$

Moreover, for large enough constant c_0, we have

$$\sum_{k=1}^{K}\int_{\mathbb{R}^{D_Y}}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)}\frac{\|w\|+\sqrt{D_Y}}{\sigma_t^2}\frac{1}{(2\pi\sigma_t^2)^{\frac{D_Y}{2}}}\cdot\mathbf{1}\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\geq c_0\sigma_{t_{i-1}}\sqrt{\log n},\|w\|\leq c\sqrt{\log n}\right)$$
$$\cdot\exp\left(-\frac{\|w-m_tG^*_{[k]}(z,x)\|^2}{2\sigma_t^2}\right)\cdot\widetilde{\rho}_k(x,G^*_{[k]}(z,x))v^*_{[k]}(z|x)\,\mathrm{d}z\,\mathrm{d}w$$
$$\leq\sum_{k=1}^{K}\frac{c\sqrt{\log n}+\sqrt{D_Y}}{\sigma_t^2}\exp\left(-\frac{c_0^2\sigma_{t_{i-1}}^2\log n}{4\sigma_t^2}\right)\int_{\mathbb{R}^{D_Y}}\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)}v^*_{[k]}(z|x)\cdot\mathbf{1}\left(\|w\|\leq c\sqrt{\log n}\right)\mathrm{d}z\,\mathrm{d}w\leq\frac{1}{n^2}$$

Therefore, we have

$$\int\left\|\nabla\log p_{t|x}(w)\right\|^2p_{t|x}(w)\cdot 1\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\geq c_0\sigma_{t_{i-1}}\sqrt{\log n}\right)\,\mathrm{d}w\leq c_1\frac{1}{n^2}.$$

Similarly, we can show

$$\int\|S(w,x,t)\|^2p_{t|x}(w)\cdot 1\left(\mathrm{dist}(w,\mathcal{M}_{Y|x})\geq c_0\sigma_{t_{i-1}}\sqrt{\log n}\right)\,\mathrm{d}x$$
$$\leq\int c^2\frac{\log n}{\sigma_t^2}p_{t|x}(w)\cdot 1\left(\mathrm{dist}(x,\mathcal{M}_{Y|x})\geq c_0\sigma_{t_{i-1}}\sqrt{\log n}\right)\,\mathrm{d}x\leq c^2c_1\frac{1}{n^2}.$$

The first statement is then proved. For the second statement. Denote $\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w)$ as any point inside $\arg\min_{y\in\mathcal{M}_{Y|x}}\|w-y\|$. Then for any $x\in\mathcal{M}_X$, $w\in\mathbb{R}^{D_Y}$ with $\mathrm{dist}(w,\mathcal{M}_{Y|x})\leq c_0\sigma_{t_{i-1}}\sqrt{\log n}$, we denote $\omega=(x,\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w))$, and use the notation $G^\omega:\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)\times U_X^\omega\to U_Y^\omega$ and v^ω in Assumption D. Then there exists a constant L_1 so that for any $z\in\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)$,

$$\|G^\omega(z,x)-G^\omega(0,x)\|\leq L_1\|z\|,$$

and by Lemma B.2, we have

$$(2\pi\sigma_t^2)^{\frac{D}{2}}p_{t|x}(w)=\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\right]$$
$$\geq\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot\mathbf{1}\left(y\in\mathbb{B}_{\mathcal{M}_{Y|x}}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(w),r_0\sigma_t)\right)\right]$$
$$=\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)}\exp\left(-\frac{\|w-m_tG^\omega(z,x)\|^2}{2\sigma_t^2}\right)\cdot\mathbf{1}\left(G^\omega(z,x)\in\mathbb{B}_{\mathcal{M}_{Y|x}}(G^\omega(0,x),r_0\sigma_t)\right)v^\omega(z|x)\,\mathrm{d}z$$
$$\geq\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)}\exp\left(-\frac{(c_0\sigma_{t_{i-1}}\sqrt{\log n}+r_0\sigma_t+(1-m_t))^2}{2\sigma_t}\right)\cdot\mathbf{1}(G^\omega(z,x)\in\mathbb{B}_{\mathcal{M}_{Y|x}}(G^\omega(0,x),r_0\sigma_t))v^\omega(z|x)\,\mathrm{d}z$$
$$\geq\int_{\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1\wedge\frac{r_0\sigma_t}{L_1})}\exp\left(-\frac{(c_0\sigma_{t_{i-1}}\sqrt{\log n}+r_0\sigma_t+(1-m_t))^2}{2\sigma_t}\right)v^\omega(z|x)\,\mathrm{d}z$$
$$\geq n^{-c_2}.$$

Therefore, for any $x\in\mathcal{M}_X$ and $w\in\mathbb{R}^{D_Y}$ with $\mathrm{dist}(w,\mathcal{M}_{Y|x})\leq c_0\sigma_{t_{i-1}}\sqrt{\log n}$,

$$\|\nabla\log p_{t|x}(w)\|=\left\|\frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot-\frac{(w-m_ty)}{\sigma_t^2}\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\right]}\right\|$$
$$\leq\left\|\frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot-\frac{(w-m_ty)}{\sigma_t^2}\cdot\mathbf{1}(\|w-m_ty\|\leq c_3\sigma_t\sqrt{\log n})\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\right]}\right\|$$
$$+\left\|\frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot-\frac{(w-m_ty)}{\sigma_t^2}\cdot\mathbf{1}(\|w-m_ty\|>c_3\sigma_t\sqrt{\log n})\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\right]}\right\|,$$

when c_3 is large enough, we have

$$\left\|\frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w-m_ty)}{\sigma_t^2}\cdot \mathbf{1}(\|w-m_ty\|>c_3\sigma_t\sqrt{\log n})\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\right]}\right\|$$
$$\le n^{c_2}\left\|\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w-m_ty)}{\sigma_t^2}\cdot \mathbf{1}(\|w-m_ty\|>c_3\sigma_t\sqrt{\log n})\right]\right\|\lesssim \frac{1}{n},$$

so

$$\|\nabla \log p_{t|x}(w)\|\le\left\|\frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot -\frac{(w-m_ty)}{\sigma_t^2}\cdot \mathbf{1}(\|w-m_ty\|\le c_3\sigma_t\sqrt{\log n})\right]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\left[\exp\left(-\frac{\|w-m_ty\|^2}{2\sigma_t^2}\right)\cdot \mathbf{1}(\|w-m_ty\|\le c_3\sigma_t\sqrt{\log n})\right]}\right\|+\frac{1}{n}$$
$$\lesssim \frac{\sqrt{\log n}}{\sigma_t}\asymp\frac{\sqrt{\log n}}{\sigma_{t_{i-1}}}.$$

We can then get the desired statement by combining all pieces.

C.4.1 Proof of Lemma C.5

By Assumption D, there exists constant L, L_1, L_1' that for any $\omega=(x^*,y^*)\in\mathcal{M}$ and any $x,x'\in U_X^\omega$, $z,z'\in\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)$,

$$\|G^\omega(z,x)-G^\omega(z',x')\|\le L_1(\|z-z'\|+\|x-x'\|^{\beta_X\wedge 1}),$$
$$\|G^\omega(z,x)-G^\omega(z',x)-J_{G^\omega(\cdot,x)}(z')(z-z')\|\le L_1\|z-z'\|^2,$$

and

$$\|z-z'\|=\|Q_x^\omega(G^\omega(z,x))-Q_x^\omega(G^\omega(z',x))\|\le L\|G^\omega(z,x)-G^\omega(z',x)\|.$$

Therefore, for any $z'\in\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)$ and unit vector $h\in\mathbb{R}^{d_Y}$, there exists a number a_0 so that for any $0<a\le a_0$ and $z=z'+ah\in\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)$, it holds that

$$\begin{aligned}a\|J_{G^\omega(\cdot,x)}(z')h\|&\ge\|G^\omega(z,x)-G^\omega(z',x)\|-L_1\|z-z'\|^2\\&\ge\frac{1}{L}\|z-z'\|-L_1\|z-z'\|^2\\&=\frac{a}{L}-L_1a^2.\end{aligned}$$

By setting $a\to 0$, we have for any unit vector h

$$\|J_{G^\omega(\cdot,x)}(z')h\|\ge\frac{1}{L}.$$

The proof for the first statement is then completed. For the second and third statement, without loss of generality, we assume $L,L_1\ge 1$ and $r_0,r\le 1$, then we choose

$$r=\left(\frac{r_0}{8L_1^2L}\right)^{\frac{1}{\beta_X\wedge 1}}\wedge\left(\frac{r_1}{4L_1L}\right)^{\frac{1}{\beta_X\wedge 1}}\wedge\frac{1}{3}\left(\frac{r_0}{4L_1}\right)^{\frac{1}{\beta_X\wedge 1}},$$

and $\overline{r}=Lr+LL_1r^{\beta_X\wedge 1}$. For the second statement, for any $k\in[K]$, if $\|x-x_k^*\|\le r$ and $\|y-y_k^*\|\le r$, we have

$$\begin{aligned}\|Q_x^{(x_k^*,y_k^*)}(y)\|&=\|Q_x^{(x_k^*,y_k^*)}(y)-Q_x^{(x_k^*,y_k^*)}(G^{(x_k^*,y_k^*)}(0,x))\|\\&\le L\|y-G^{(x_k^*,y_k^*)}(0,x)\|\\&\le L\|y-y_k^*\|+L\|G^{(x_k^*,y_k^*)}(0,x_k^*)-G^{(x_k^*,y_k^*)}(0,x)\|\\&\le Lr+LL_1r^{\beta_X\wedge 1}=\overline{r}\le\frac{r_1}{2}\wedge\frac{r_0}{4L_1}.\end{aligned}\tag{30}$$

For the last statement, notice that for any $(x, y) \in \mathcal{M}$, there exists $k \in [K]$, so that $\|x - x_k^*\| \leq r$, and $\|y - y_k^*\| \leq r$, and there exists $x^* \in \mathcal{N}_{\varepsilon_2}^X$ so that $\|x - x^*\| \leq \varepsilon_2 \leq r$. So we have

$$\|x^* - x_k^*\| \leq \|x - x^*\| + \|x - x_k^*\| \leq 2r,$$

which implies $k \in \mathcal{K}_{x^*}$. Then by equation (30), there exists $z^* \in \mathcal{N}_{\varepsilon_1}^Z$ so that $\|z^* - Q_x^{(x_k^*, y_k^*)}(y)\| \leq \varepsilon_1$, and thus

$$\|G^{(x_k^*, y_k^*)}(z^*, x) - y\| = \|G^{(x_k^*, y_k^*)}(z^*, x) - G^{(x_k^*, y_k^*)}(Q_x^{(x_k^*, y_k^*)}(y), x)\| \leq L_1 \varepsilon_1.$$

Proof of the second and third statement is then completed. For the last statement, if $z \in \mathbb{B}_{\mathbb{R}^{d_Y}}(0, \overline{r})$ and

$$\|x - x_k^*\| \leq \|x - x^*\| + \|x^* - x_k^*\| \leq \varepsilon_2 + 2r \leq 3r,$$

then

$$\begin{aligned} \|G^{(x_k^*, y_k^*)}(z, x) - y_k^*\| &= \|G^{(x_k^*, y_k^*)}(z, x) - G^{(x_k^*, y_k^*)}(0, x_k^*)\| \\ &\leq L_1 \|z\| + L_1 \|x - x_k^*\|^{\beta_X \wedge 1} \\ &\leq L_1 \overline{r} + L_1 (3r)^{\beta_Y \wedge 1} \\ &\leq \frac{r_0}{2}. \end{aligned}$$

C.4.2 Proof of Lemma C.6

Consider $x \in \mathcal{M}_X$ and $w \in \mathbb{R}^{D_Y}$ so that $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \leq c_0 \sigma_{\underline{t}} \sqrt{\log n}$. Then there exists $y \in \mathcal{M}_{Y|x}$, $j_2 \in [J_2]$, $j_1 \in [J_1]$, $k \in \mathcal{K}_{\widetilde{x}_{j_2}}$, so that $\|\widetilde{x}_{j_2} - x\| \leq \varepsilon_2$, $\|G_{[k]}^*(\widetilde{z}_{j_1}, x) - y\| \leq L_1 \varepsilon_1$, and $\|w - y\| \leq c_0 \sigma_{\underline{t}} \sqrt{\log n}$. So we have

$$\|w - G_{[k]}^*(\widetilde{z}_{j_1}, x)\| \leq L_1 \varepsilon_1 + c_0 \sigma_{\underline{t}} \sqrt{\log n}.$$

Then notice that $G_{[k]}^*(z, x)$ is $C_{D_Y}^{\beta_Y, \beta_X}$-smooth, let

$$G_{[k]}^*|_{\widetilde{x}}(z, x) = \sum_{\substack{j \in \mathbb{N}_0^{d_X} \\ |j| < \beta_X}} \frac{G_{[k](0,j)}^*(z, \widetilde{x})}{j!} (x - \widetilde{x})^j,$$

we have

$$\|G_{[k]}^*|_{\widetilde{x}_{j_2}}(z, x) - G_{[k]}^*(z, x)\| \leq L_1 \|\widetilde{x}_{j_2} - x\|^{\beta_X} \leq L_1 \varepsilon_2^{\beta_X},$$

and therefore,

$$\|w - G_{[k]}^*|_{\widetilde{x}_{j_2}}(\widetilde{z}_{j_1}, x)\| \leq L_1 \varepsilon_1 + c_0 \sigma_{\underline{t}} \sqrt{\log n} + L_1 \varepsilon_2^{\beta_X} \leq 2 L_1 \varepsilon_1 + c_0 \sigma_{\underline{t}} \sqrt{\log n}.$$

Then define

$$\widetilde{\rho}(x) = \begin{cases} 1 & |x| < 1 \\ 0 & |x| > 2 \\ 2 - |x| & 1 < |x| \leq 2 \end{cases}$$

For any $j_1 \in [J_1]$ and $j_2 \in [J_2]$, $k \in \mathcal{K}_{\widetilde{x}_{j_2}}$, define

$$\widetilde{\rho}_{kj_1j_2}(x, w) = \widetilde{\rho}\left(\frac{\|x - \widetilde{x}_{j_2}\|^2}{\varepsilon_2^2}\right) \widetilde{\rho}\left(\frac{\|w - G_{[k]}^*|_{\widetilde{x}_{j_2}}(\widetilde{z}_{j_1}, x)\|^2}{(c_0 \sigma_{\underline{t}} \sqrt{\log n} + 2 L_1 \varepsilon_1)^2}\right),$$

$$\rho_{kj_1j_2}(x, w) = \frac{\widetilde{\rho}_{kj_1j_2}(x, w)}{\sum_{j_1 \in [J_1]} \sum_{j_2 \in [J_2]} \sum_{k \in \mathcal{K}_{\widetilde{x}_{j_2}}} \widetilde{\rho}_{kj_1j_2}(x, w)}.$$

Then if $\rho_{kj_1j_2}(x,w) \neq 0$ and if $\rho_{kj_1'j_2'}(x,w) \neq 0$, we have

$$\|\widetilde{x}_{j_2} - \widetilde{x}_{j_2'}\| \leq \|x - \widetilde{x}_{j_2'}\| + \|x - \widetilde{x}_{j_2}\| \leq 2\sqrt{2}\varepsilon_2,$$

and

$$\begin{aligned}
\|\widetilde{z}_{j_1} - \widetilde{z}_{j_1'}\| &\leq L\|G^*_{[k]}(\widetilde{z}_{j_1}, x) - G^*_{[k]}(\widetilde{z}_{j_1'}, x)\| \\
&\leq L\|G^*_{[k]}|_{\widetilde{x}_{j_2}}(\widetilde{z}_{j_1}, x) - G^*_{[k]}|_{\widetilde{x}_{j_2'}}(\widetilde{z}_{j_1'}, x)\| + 2LL_1\varepsilon_2^{\beta_X} \\
&\leq L\|w - G^*_{[k]}|_{\widetilde{x}_{j_2}}(\widetilde{z}_{j_1}, x)\| + L\|w - G^*_{[k]}|_{\widetilde{x}_{j_2'}}(\widetilde{z}_{j_1'}, x)\| + 2LL_1\varepsilon_2^{\beta_X} \\
&\leq 2\sqrt{2}Lc_0\sigma_{\underline{t}}\sqrt{\log n} + 2L_1\varepsilon_1 + 2LL_1\varepsilon_2^{\beta_X} \\
&\leq (2\sqrt{2}Lc_0 + 2L_1 + 2LL_1)\varepsilon_1.
\end{aligned}$$

So for any $x \in \mathcal{M}_X$ and $w \in \mathbb{R}^{D_Y}$, there are only constant-order number of k, j_1, j_2 so that $\rho_{kj_1j_2}(x,w) \neq 0$. Then we can write

$$\nabla \log p_{t|x}(w) = \sum_{j_1 \in [J_1]} \sum_{j_2 \in [J_2]} \sum_{k \in \mathcal{K}_{\widetilde{x}_{j_2}}} \nabla \log p_{t|x}(w) \cdot \rho_{kj_1j_2}(x,w).$$

By Lemma C.9 and C.10, and the fact that $G^*_{[k]}|_{\widetilde{x}_{j_2}}(\widetilde{z}_{j_1}, x)$ is polynomial function of x, we construct the following neural networks:

1. For $j_1 \in [J_1]$, $j_2 \in [J_2]$ and $k \in \mathcal{K}_{\widetilde{x}_{j_2}}$, we approximate $\widetilde{\rho}_{kj_1j_2}(x,w)$ by $\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w) \in \Phi(H,W,R,B)$ with $H = \Theta(\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log n)$ and $B = \exp(\Theta(\log n))$.
2. We approximate $\frac{1}{x}$ by $\phi_{rec}(x) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n)$, $\|W\|_\infty = \Theta(\log^3 n)$, $R = \Theta(\log^4 n)$ and $B = \exp(\Theta(\log^2 n))$.
3. We approximate $x \cdot y$ by $\phi_{mult}(x,y) \in \Phi(H,W,R,B)$ with $H = \Theta(\log n)$, $\|W\|_\infty = \Theta(\log n)$, $R = \Theta(\log n)$ and $B = \exp(\Theta(\log n))$.

We have for any $x \in \mathcal{M}_X$ and $w \in \mathbb{R}^{D_Y}$ with $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \leq c_0\sigma_{\underline{t}}\sqrt{\log n}$,

$$
\begin{aligned}
&\Bigg\| \sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \nabla \log p_{t|x}(w)\cdot \rho_{kj_1j_2}(x,w) \\
&-\phi_{muti}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi_{muti}\left(\phi^*_{kj_1j_2}(w,x,t),\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\right),\phi_{rec}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\right)\right)\Bigg\|_\infty \\
&\le \left\| \sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \nabla \log p_{t|x}(w)\cdot \rho_{kj_1j_2}(x,w) - \sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi^*_{kj_1j_2}(w,x,t)\cdot\rho_{kj_1j_2}(x,w)\right\|_\infty \\
&+\Bigg\| \sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi^*_{kj_1j_2}(w,x,t)\cdot\widetilde{\rho}_{kj_1j_2}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\widetilde{\rho}_{kj_1j_2}(x,w)\right)^{-1} \\
&\quad-\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi^*_{kj_1j_2}(w,x,t)\cdot\widetilde{\rho}_{kj_1j_2}(x,w)\cdot\phi_{rec}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\widetilde{\rho}_{kj_1j_2}(x,w)\right)\Bigg\|_\infty \\
&+\Bigg\| \sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi^*_{kj_1j_2}(w,x,t)\cdot\widetilde{\rho}_{kj_1j_2}(x,w)\cdot\phi_{rec}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\widetilde{\rho}_{kj_1j_2}(x,w)\right) \\
&-\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi^*_{kj_1j_2}(w,x,t)\cdot\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\cdot\phi_{rec}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\widetilde{\rho}_{kj_1j_2}(x,w)\right)\Bigg\|_\infty \\
&+\Bigg\| \sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi^*_{kj_1j_2}(w,x,t)\cdot\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\cdot\phi_{rec}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\widetilde{\rho}_{kj_1j_2}(x,w)\right) \\
&-\phi_{muti}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}} \phi_{muti}\left(\phi^*_{kj_1j_2}(w,x,t),\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\right),\phi_{rec}\left(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\right)\right)\Bigg\|_\infty \\
&\lesssim \varepsilon+\frac{1}{n}.
\end{aligned}
$$

Finally, by concatenation and parallelization of neural networks (see for example, Lemmas F.1-F.3 in [2]), there exists $\phi_{score}(x)\in\Phi(H_1,W_1,S_1,B_1,\Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}}))$ with $H_1=\Theta(H+\log^2 n)$, $\|W_1\|_\infty=\Theta(J_1J_2(\|W\|_\infty+\log n)+\log^3 n)$, $S_1=\Theta(J_1J_2(S+\log n)+\log^4 n)$ and $B_1=\exp(\Theta(\log^2 n))\vee B$ so that

$$
\begin{aligned}
&\phi_{score}(x)=\max\Bigg(-c_2\frac{\sqrt{\log n}}{\sigma_{\underline{t}}},\min\Bigg(c_2\frac{\sqrt{\log n}}{\sigma_{\underline{t}}}, \\
&\phi_{muti}\Big(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\phi_{muti}\Big(\phi^*_{kj_1j_2}(w,x,t),\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\Big),\phi_{rec}\Big(\sum_{j_1\in[J_1]}\sum_{j_2\in[J_2]}\sum_{k\in\mathcal{K}_{\widetilde{x}_{j_2}}}\phi_{\widetilde{\rho}_{kj_1j_2}}(x,w)\Big)\Big)\Bigg)\Bigg),
\end{aligned}
$$

where the $\max$ and $\min$ functions are applied elementwise to vectors. The result is then follows from the fact that $\|\nabla\log p_{t|x}(w)\|_\infty\le c_2\frac{\sqrt{\log n}}{\sigma_{\underline{t}}}$ when $x\in\mathcal{M}_X$ and $\mathrm{dist}(w,\mathcal{M}_{Y|x})\le c_0\sigma_{\underline{t}}\sqrt{\log n}$.

C.4.3 Proof of Lemma C.11

Recall

$$G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x) = \sum_{(j_1,j_2)\in\mathcal{J}^{d_Y,D_X}_{\beta_Y,\beta_X}} \frac{G^*_{[k](j_1,j_2)}(\widetilde{z},\widetilde{x})}{j_1!j_2!}(z-\widetilde{z})^{j_1}(x-\widetilde{x})^{j_2},$$

For any $l\in[d_Y]$, denotes $\mathbf{1}_l$ as the d_Y-dimensional vector in which the lth element being 1 and other elements being 0, by $\beta_Y\geq 2$, we have

$$\|\frac{\partial G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x)}{\partial z_l} - G^*_{[k](\mathbf{1}_l,0)}(\widetilde{z},\widetilde{x})\| \lesssim \|z-\widetilde{z}\| + \|x-\widetilde{x}\|^{\beta_X/2}.$$

Then notice that for any $z\in\mathbb{B}_{\mathbb{R}^{d_Y}}(0,r_1)$,

$$\lambda_{\min}(J_{G^*_{[k]}(\cdot,x)}(z)^T J_{G^*_{[k]}(\cdot,x)}(z)) \geq \frac{1}{L},$$

there exists a constant r_2 so that for any $z\in\mathbb{B}_{\mathbb{R}^{d_Y}}(\widetilde{z},r_2)$ and $x\in\mathbb{B}_{\mathcal{M}_X}(\widetilde{x},(\sigma_{\underline{t}}\sqrt{\log n})^{\frac{1}{\beta_X}})$,

$$\lambda_{\min}(J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(z)^T J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(z)) \geq \frac{1}{2L}.$$

Let $h(w,x,z) = (J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(z))^T(w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x))$. Then we can write the Jacobian of h with respect to z as

$$J_{h(w,x,\cdot)}(z) = -J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(z)^T J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(z) + \sum_{l=1}^{D_Y}(w_l - G^*_{[k],l}|_{(\widetilde{z},\widetilde{x})}(z,x))\mathcal{H}_l(z,x),$$

where $G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z,x) = (G^*_{[k],1}|_{(\widetilde{z},\widetilde{x})}(z,x),\cdots,G^*_{[k],D_Y}|_{(\widetilde{z},\widetilde{x})}(z,x))$ and $\mathcal{H}_l(z,x)$ denotes the Hessian matrix of $G^*_{[k],l}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)$ at z. Then denote

$$g(w,x,z) = z - (J_{h(w,x,\cdot)}(z))^{-1}h(w,x,z).$$

Note that for any $w\in\mathbb{R}^{D_Y}$ satisfying $\|w - G^*_{[k]}(\widetilde{z},x)\| \lesssim (\sigma_{\underline{t}}\vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}$ and $x\in\mathbb{B}_{\mathcal{M}_X}(\widetilde{x},(\sigma_{\underline{t}}\sqrt{\log n})^{\frac{1}{\beta_X}})$, we have

$$\|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\widetilde{z},x)\| \leq \|w - G^*_{[k]}(\widetilde{z},x)\| + C\|x-\widetilde{x}\|^{\beta_X} \lesssim (\sigma_{\underline{t}}\vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}.$$

So by $\lambda_{\min}(J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(z)^T J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(z)) \geq \frac{1}{2L}$ and the C^∞-smoothness of h, when n is large enough, the exist positive constants r_3, L_2, L_3 so that when $\|z-\widetilde{z}\|\leq r_3$ and $\|x-\widetilde{x}\|\leq(\sigma_{\underline{t}}\sqrt{\log n})^{\frac{1}{\beta_X}}$,

$$-L_2 I_{d_Y} \preccurlyeq J_{h(w,x,\cdot)}(z) \preccurlyeq -L_3 I_{d_Y}.$$

Furthermore, by

$$\|h(w,x,\widetilde{z})\| \lesssim (\sigma_{\underline{t}}\vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}.$$

we have

$$\|g(w,x,\widetilde{z}) - \widetilde{z}\| = \mathcal{O}(\|h(w,x,\widetilde{z})\|) \lesssim (\sigma_{\underline{t}}\vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n},$$

and

$$\begin{aligned}\|h(w,x,g(w,x,\widetilde{z}))\| &= \left\|h\left(w,x,\widetilde{z} - (J_{h(w,x,\cdot)}(\widetilde{z}))^{-1}h(w,x,\widetilde{z})\right)\right\| \\ &= \left\|h(w,x,\widetilde{z}) - J_{h(w,x,\cdot)}(\widetilde{z})(J_{h(w,x,\cdot)}(\widetilde{z}))^{-1}h(w,x,\widetilde{z})\right\| + \mathcal{O}(\|h(w,x,\widetilde{z}))\|^2) \\ &\lesssim \left((\sigma_{\underline{t}}\vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^2.\end{aligned}$$

Similarly, define

$$\overline{g}(w,x) = \underbrace{g(w,x,g(w,x,\circ g(w,x,\circ\cdots\circ g(w,x,g(w,x,g(}_{\lceil \log_2(2\beta_Y)\rceil} w,x,\widetilde{z})))))),$$

we can obtain

$$\|\overline{g}(w,x)-\widetilde{z}\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n},$$

and

$$\|h(w,x,\overline{g}(w,x))\| \lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y}.$$

Then we approximate $\overline{g}(w,x)$ by the neural network. Notice that by Cayley-Hamilton theorem, for $A \in \mathbb{R}^{d\times d}$, denote S_k as the trace of A^k and B_k as the kth complete exponential Bell polynomial.[2] We can write

$$\det(A) = \frac{1}{d!}B_d(S_1,-1!S_2,\cdots,(-1)^{d-1}(n-1)!S_d)$$

$$A^{-1} = \frac{1}{\det(A)}\sum_{k=0}^{d-1}(-1)^{d+k-1}\frac{A^{d-k-1}}{k!}B_i(S_1,-1!S_2,\cdots,(-1)^{k-1}(k-1)!S_k).$$

By Lemmas C.9 and C.10, there exists $\phi_g(w,x,z) \in \Phi(H,W,R,B)$ and $\phi_{g(\cdot,\widetilde{z})}(w,x) \in \Phi(H_1,W_1,R_1,B_1)$ with $H \asymp H_1 = \Theta(\log^2 n)$, $\|W\|_\infty \asymp \|W_1\|_\infty = \Theta(\log^3 n)$, $R \asymp R_1 = \Theta(\log^4 n)$ and $B \asymp B_1 = \exp(\Theta(\log^2 n))$ so that for any $x \in \mathcal{M}_X$ satisfying $\|x-\widetilde{x}\| \lesssim (\sigma_{\underline{t}}\sqrt{\log n})^{\frac{1}{\beta_X}}$, $w \in \mathbb{R}^{D_Y}$ satisfying $\|w - G^*_{[k]}(\widetilde{z},x)\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}$ and $\|z\| \le r_3$,

$$\|\phi_g(w,x,z) - g(w,x,z)\| \lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y}.$$

and

$$\|\phi_{g(\cdot,\widetilde{z})}(w,x) - g(w,x,\widetilde{z})\| \lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y}.$$

Furthermore,

$$\Bigg\| \underbrace{g(w,x,g(w,x,\circ g(w,x,\circ\cdots\circ g(w,x,g(w,x,g(}_{\lceil \log_2(2\beta_Y)\rceil} w,x,\widetilde{z})))))) - \underbrace{\phi_g(w,x,\phi_g(w,x,\circ\phi_g(w,x,\circ\cdots\circ\phi_g(w,x,\phi_g(w,x,\phi_{g(\cdot,\widetilde{z})}(}_{\lceil \log_2(2\beta_Y)\rceil} w,x)))))) \Bigg\|$$
$$\lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y+d_Y+d_X\frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y}.$$

So by concatenation and parallelization of neural networks, there exists $\phi_p(w,x) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^2 n)$, $\|W\|_\infty = \Theta(\log^3 n)$, $R = \Theta(\log^4 n)$ and $B = \exp(\Theta(\log^2 n))$ so that for

[2] $B_k(x_1,\dots,x_k) = \sum_{w=1}^{k} B_{k,w}(x_1,x_2,\dots,x_{k-w+1})$ with $B_{k,w}(x_1,x_2,\dots x_{k-w+1}) = \sum_{\substack{j_1+\dots+j_{k-w+1}=w \\ j_1+2j_2+\dots+(k-w+1)j_{k-w+1}=k}} \frac{k!}{j_1!j_2!\dots j_{k-w+1}!}\left(\frac{x_1}{1!}\right)^{j_1}\left(\frac{x_2}{2!}\right)^{j_2}\cdots\left(\frac{x_{k-w+1}}{k-w+1!}\right)^{j_{k-w+1}}$

any $x \in \mathcal{M}_X$ satisfying $\|x - \widetilde{x}\| \lesssim (\sigma_{\underline{t}}\sqrt{\log n})^{\frac{1}{\beta_X}}$, $w \in \mathbb{R}^{D_Y}$ satisfying $\|w - G^*_{[k]}(\widetilde{z}, x)\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}$,

$$\|\phi_p(w, x) - \overline{g}(w, x)\| \lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y}.$$

So we have

$$\begin{aligned}
&\left\|\left\langle J_{G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\cdot,x)}(\phi_p(w,x)), w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\phi_p(w,x),x)\right\rangle\right\| \\
&= \|h(w, x, \phi_p(w,x))\| \lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y}.
\end{aligned}$$

The proof of the first statement is completed. Then for the second statement, define

$$f(w, x, z) = \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(z, x)\|^2.$$

Then we have

$$J_{f(w,x,\cdot)}(z) = -2h(w, x, z)$$

and the Hessian matrix of $f(w, x, \cdot)$ at z is $-2J_{h(w,x,\cdot)}(z)$. Then we denote

$$\overline{g}_k(w, x) = \underbrace{g(w, x, g(w, x, \circ g(w, x, \circ \cdots \circ g(w, x, g(w, x, g(}_{k}w, x, \widetilde{z})))))).$$

Then for any $x \in \mathcal{M}_X$ satisfying $\|x - \widetilde{x}\| \lesssim (\sigma_{\underline{t}}\sqrt{\log n})^{\frac{1}{\beta_X}}$, $w \in \mathbb{R}^{D_Y}$ satisfying $\|w - G^*_{[k]}(\widetilde{z}, x)\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}$, we have $\overline{z} = \lim_{k\to\infty} g_k(w, x)$ exists and

$$\|\overline{z} - \phi_p(w, x)\| \lesssim \left((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}\right)^{2\beta_Y} \lesssim \sigma_{\underline{t}}\sqrt{\log n}$$

$$\|\overline{z} - \widetilde{z}\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n},$$

$$J_{f(w,x,\cdot)}(\overline{z}) = 0.$$

Therefore, for any $\|z - \widetilde{z}\| \le r_3$,

$$f(w, x, z) - f(w, x, \overline{z}) \ge 2L_3\|z - \overline{z}\|^2.$$

Then if

$$\|Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x) - \overline{z}\| \ge C_2\sigma_{\underline{t}}\sqrt{\log n},$$

for a large enough C_2, we have,

$$\|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\|^2 - \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\overline{z}, x)\|^2 \ge 2L_3C_2^2\sigma_{\underline{t}}^2\log n.$$

Moreover, notice that $\|w - G^*_{[k]}(\widetilde{z}, x)\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}$ and $\mathrm{dist}(w, \mathcal{M}_{Y|x}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}$, we have

$$\|\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega) - G^*_{[k]}(\widetilde{z}, x)\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n},$$

and

$$\|Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x) - \widetilde{z}\| \lesssim (\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n}.$$

Therefore

$$
\begin{aligned}
&\|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\overline{z}, x)\| \\
&\leq \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\| \\
&\leq \|w - G^*_{[k]}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\| + ((\sigma_{\underline{t}} \vee n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}})\sqrt{\log n})^{\beta_Y} + \sigma_{\underline{t}}\sqrt{\log n} \\
&\leq C_3 \sigma_{\underline{t}} \sqrt{\log n}.
\end{aligned}
$$

So we have

$$
\begin{aligned}
&\|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\| - \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\overline{z}, x)\| \\
&= \frac{\|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\|^2 - \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\overline{z}, x)\|^2}{\|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\| + \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\overline{z}, x)\|} \geq \frac{L_3 C_2^2}{C_3} \sigma_{\underline{t}} \sqrt{\log n}.
\end{aligned}
$$

Then notice that

$$
\|w - G^*_{[k]}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\| \geq \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\| - C\sigma_{\underline{t}}\sqrt{\log n},
$$

and

$$
\|w - G^*_{[k]}(\overline{z}, x)\| \leq \|w - G^*_{[k]}|_{(\widetilde{z},\widetilde{x})}(\overline{z}, x)\| + C\sigma_{\underline{t}}\sqrt{\log n},
$$

when C_2 is large enough, we have

$$
\|w - G^*_{[k]}(\overline{z}, x)\| < \|w - G^*_{[k]}(Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x), x)\|,
$$

which cause contradiction. So

$$
\begin{aligned}
&\|Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x) - \phi_p(w, x)\| \\
&\leq \|Q^*_{[k]}(\mathrm{Proj}_{\mathcal{M}_{Y|x}}(\omega), x) - \overline{z}\| + \|\phi_p(w, x) - \overline{z}\| \lesssim \sigma_{\underline{t}}\sqrt{\log n}.
\end{aligned}
$$

C.4.4 Proof of lemma C.12

Let $\phi(x, \mu, \Sigma)$ denotes the density function of $\mathcal{N}(\mu, \Sigma)$, we have

$$
\begin{aligned}
&\mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\left[\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\|^2\right] \\
&= \mathbb{E}_{x\sim\mu_X^*}\left[\int \left\|S(w_t,x,t)-\nabla\log p_{t|x}(w_t)\right\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t\right] \\
&= \mathbb{E}_{x\sim\mu_X^*}\Bigg[\int \|S(w_t,x,t)\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t + \int \left\|\nabla\log p_{t|x}(w_t)\right\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t \\
&\qquad - 2\int S(w_t,x,t)^T\,\nabla\log p_{t|x}(w_t)\,p_{t|x}(w_t)\,\mathrm{d}w_t\Bigg] \\
&= \mathbb{E}_{x\sim\mu_X^*}\Bigg[\int \|S(w_t,x,t)\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t + \int \left\|\nabla\log p_{t|x}(w_t)\right\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t \\
&\qquad - 2\int S(w_t,x,t)^T\,\nabla p_{t|x}(w_t)\,\mathrm{d}w_t\Bigg] \\
&= \mathbb{E}_{x\sim\mu_X^*}\Bigg[\int \|S(w_t,x,t)\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t + \int \left\|\nabla\log p_{t|x}(w_t)\right\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t \\
&\qquad - 2\int S(w_t,x,t)^T\,\nabla\Big(\mathbb{E}_{y\sim\mu_{Y|x}^*}[\phi(w_t,m_t y,\sigma_t^2 I_{D_y})]\Big)\mathrm{d}w_t\Bigg] \\
&= \mathbb{E}_{x\sim\mu_X^*}\Bigg[\int \|S(w_t,x,t)\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t + \int \left\|\nabla\log p_{t|x}(w_t)\right\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t \\
&\qquad - 2\int S(w_t,x,t)^T\,\mathbb{E}_{y\sim\mu_{Y|x}^*}[\nabla\phi(w_t,m_t y,\sigma_t^2 I_{D_y})]\mathrm{d}w_t\Bigg] \\
&= \mathbb{E}_{x\sim\mu_X^*}\Bigg[\int \|S(w_t,x,t)\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t + \int \left\|\nabla\log p_{t|x}(w_t)\right\|^2 p_{t|x}(w_t)\,\mathrm{d}w_t \\
&\qquad - 2\int S(w_t,x,t)^T\,\mathbb{E}_{y\sim\mu_{Y|x}^*}\left[\nabla\log\phi(w_t,m_t y,\sigma_t^2 I_{D_y})\cdot\phi(w_t,m_t y,\sigma_t^2 I_{D_y})\right]\mathrm{d}w_t\Bigg] \\
&= \mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\Big[\|S(w_t,x,t)\|^2 + \left\|\nabla\log p_{t|x}(w_t)\right\|^2 \\
&\qquad - 2S(w_t,x,t)^T\,\nabla\log\phi(w_t,m_t y,\sigma_t^2 I_{D_y})\Big] \\
&= \mathbb{E}_{x\sim\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\left[\|S(w_t,x,t)-\frac{m_t Y-w_t}{\sigma_t^2}\|^2\right] \\
&\quad + \mathbb{E}_{\mu_X^*}\mathbb{E}_{y\sim\mu_{Y|x}^*}\mathbb{E}_{w_t\sim\mathcal{N}(m_t y,\sigma_t^2 I_{D_Y})}\left[\left\|\nabla\log p_{t|x}(w_t)\right\|^2 - \left\|\frac{m_t Y-w_t}{\sigma_t^2}\right\|^2\right].
\end{aligned}
$$

C.4.5 Proof of Lemma C.13

For $G_i^* = \{g(x,y) = \ell_i(x,y,S) - \ell_i(x,y,S_i^*) \,:\, S\in\mathcal{S}_i\}$, it holds that

$$\sup_{g\in G_i^*}\sup_{(x,y)\in\mathcal{M}} |g(x,y)| \lesssim (\log n)^2.$$

Define

$$Z_n(\delta, G_i^*) = \sup_{\substack{g\in G_i^*\\ \|g\|_2\le\delta}}\left|\frac{1}{n}\sum_{i=1}^n g(X_i,Y_i) - \mathbb{E}_{\mu^*}[g(x,y)]\right|.$$

Since $\frac{1}{n}\sup_{\substack{g\in G_i^*\\ \|g\|_2\le\delta}}\sum_{i=1}^n var(g(x_i)) \le \delta^2$, by the tail inequality for suprema of bounded empirical processes (see for example, Theorem 3.27 of [6]), it holds that

$$P(Z_n(\delta,G_i^*) \ge \mathbb{E}_{\mu^{*\otimes n}}[Z_n(\delta,G_i^*)] + c_0(\delta + (\log n)\sqrt{\mathbb{E}_{\mu^{*\otimes n}}[Z_n(\delta,G_i^*)]})\sqrt{t} + c_1(\log n)^2 t) \le \exp(-nt)\,. \tag{31}$$

Using the standard symmetrization (see, for example, Proposition 4.11 of [6]), we can get

$$\mathbb{E}_{\mu^{*\otimes n}}\left[Z_n(\delta, G_i^*)\right] \le \mathbb{E}_{\mu^{*\otimes n}}\mathbb{E}_{\epsilon}\left[\sup_{\substack{g\in G_i^*\\ \|g\|_2\le\delta}}\left|\frac{2}{n}\sum_{i=1}^n \epsilon_i g(X_i, Y_i)\right|\right]$$
$$= 2\overline{R}_n(\delta, G_i^*) \le 2\overline{R}_n(\delta, \overline{G}_i^*),$$

where recall that $\overline{G}_i^* = \{ag | a \in (0,1], g \in G_i^*\}$ and $\{\epsilon_i\}_{i=1}^n$ are n i.i.d. copies from Rademacher distribution, i.e. $\mathbb{P}(\epsilon_i = 1) = \mathbb{P}(\epsilon_i = -1) = \frac{1}{2}$. Therefore by $\overline{R}_n(\delta_{ni}, \overline{G}_i^*) \le \delta_{ni}^2/(\log n)^2$, it holds that

$$\forall r \ge \delta_{ni}, \quad \mathbb{E}_{\mu^{*\otimes n}}\left[Z_n(r, G_i^*)\right] \le 2\overline{R}_n(r, \overline{G}_i^*)$$
$$= 2\mathbb{E}_{\mu^{*\otimes n}}\mathbb{E}_{\varepsilon}\left[\sup_{\substack{g\in\overline{G}_i^*\\ \|\frac{\delta_{ni}}{r}g\|_2\le\delta_{ni}}} \frac{r}{\delta_{ni}}\left|\frac{1}{n}\sum_{i=1}^n \varepsilon_i \frac{\delta_{ni}}{r} g(x_i)\right|\right]$$
$$\le 2\frac{r}{\delta_{ni}}\overline{R}_n(\delta_{ni}, \overline{G}_i^*)$$
$$\le 2r\delta_{ni}/(\log n)^2.$$

Define the events

$$\mathcal{A}_0 = \{Z_n(\delta_{ni}, G_i^*) \ge c_2\delta_{ni}^2/(\log n)^2\};$$
$$\mathcal{A}_1 = \{\exists g \in G_i^*, \text{such that} \left|\frac{1}{n}\sum_{i=1}^n g(X_i, Y_i) - \mathbb{E}_{\mu^{*\otimes n}}[g(x,y)]\right| \ge c_2\delta_{ni}\|g\|_2/(\log n)^2$$
$$\text{and } \|g\|_2 \ge \delta_{ni}\}.$$

Using equation (31), there exist some constants (c_0', c_1', c_2) such that

$$P(\mathcal{A}_0) \le \frac{1}{n^2}.$$

Define $\mathcal{S}_m = \left\{2^{m-1}\delta_{ni} \le \|g\|_2 \le 2^m\delta_{ni}\right\}$ with $m = 1, \cdots M$, since $\|g\|_2 \lesssim (\log n)^2$, we have $M \lesssim \log(\frac{1}{\delta_{ni}})$.

Under $\mathcal{A}_1 \cap \mathcal{S}_m$, it holds that $Z_n(2^m\delta_{ni}, G_i^*) \ge c_2 2^{m-1}\delta_{ni}^2/(\log n)^2$. Therefore,

$$P(\mathcal{A}_1) = \sum_{m=1}^M P(\mathcal{A}_1 \cap \mathcal{S}_m) \le \frac{1}{n^2}.$$

Moreover, under $\mathcal{A}_0^c \cap \mathcal{A}_1^c$, we have

$$\sup_{g\in G_i^*} \frac{\left|\frac{1}{n}\sum_{i=1}^n g(X_i, Y_i) - \mathbb{E}_{\mu^*}[g(x,y)]\right|}{\delta_{ni} + \|g\|_2} \le c_2\delta_{ni}/(\log n)^2.$$

We can then get the desired conclusion.

D Proof of Theorem 1

Under Assumptions A and B, we can derive the following theorem for controlling the conditional score approximation error.

Lemma D.1. *For any* $t \in [\underline{t}, \overline{t}]$ *with* $1 < \frac{\overline{t}}{\underline{t}} \le 2$*:*

1. *If* $\tau \le \underline{t} < n^{-\frac{2}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}}$*, there exists a neural network* $\phi_{score}(w, x, t) \in \Phi(H, W, R, B, V)$ *satisfying*

$$\mathbb{E}_{\mu_X^*}\Big[\int_{\underline{t}}^{\bar{t}} \int_{\mathbb{R}^{D_Y}} \left\|\phi_{score}(w, x, t) - \nabla \log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\mathrm{d}t\Big] = \widetilde{\mathcal{O}}(\varepsilon_1^{2\alpha_Y} + \varepsilon_2^{2\alpha_X}),$$

where $\varepsilon_1 = n^{-\frac{1}{2\alpha_Y + d_Y + \frac{\alpha_Y}{\alpha_X} d_X}}$ *and* $\varepsilon_2 = \varepsilon_1^{\frac{\alpha_Y}{\alpha_X}}$*. Here* H*,* W*,* R*,* B *and* V *are evaluated as* $H = \Theta\left(\log^4 n\right)$*,* $\|W\|_\infty = \widetilde{\Theta}\left(\varepsilon_1^{-d_Y}\varepsilon_2^{-d_X}\right)$*,* $R = \widetilde{\Theta}\left(\varepsilon_1^{-d_Y}\varepsilon_2^{-d_X}\right)$*,* $B = \exp\left(\Theta(\log^4 n)\right)$ *and* $V = \Theta(\sqrt{\frac{\log n}{\underline{t}}})$*.*

2. *If* $n^{-\frac{2}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}} \le \underline{t} \le T$*, there exists a neural network* $\phi_{score}(w, x, t) \in \Phi(H, W, R, B, V)$ *satisfying*

$$\mathbb{E}_{\mu_X^*}\Big[\int_{\underline{t}}^{\bar{t}} \int_{\mathbb{R}^{D_Y}} \left\|\phi_{score}(w, x, t) - \nabla \log p_{t|x}(w)\right\|^2 p_{t|x}(w)\,\mathrm{d}w\mathrm{d}t\Big] = \widetilde{\mathcal{O}}(\varepsilon_2^{2\alpha_X}),$$

with $\varepsilon_2 = \widetilde{\Theta}(n^{-\frac{1}{2\alpha_X + d_X}} \underline{t}^{-\frac{d_Y}{4\alpha_X + 2d_X}})$*. Here* H*,* W*,* R*,* B *and* V *are evaluated as* $H = \Theta\left(\log^4 n\right)$*,* $\|W\|_\infty = \widetilde{\Theta}\left(\underline{t}^{-\frac{d_Y}{2}}\varepsilon_2^{-d_X}\right)$*,* $R = \widetilde{\Theta}\left(\underline{t}^{-\frac{d_Y}{2}}\varepsilon_2^{-d_X}\right)$*,* $B = \exp\left(\Theta(\log^4 n)\right)$ *and* $V = \Theta(\sqrt{\frac{\log n}{\underline{t} \wedge 1}})$*.*

Then similarly to the proof of Theorem 2, combined with Lemma C.3 for the estimation error, we can obtain the desired result.

D.1 Proof of Lemma D.1

Similar as Lemma C.4, we have the following lemma for addressing the unboundedness of the space and the score function.

Lemma D.2. *If* $\sup_{w \in \mathbb{R}^{D_Y}, x \in [-1,1]^{D_X}} \sup_{t \in [\tau, T]} [\|S(w, x, t)\|_\infty \sigma_t] \le c\sqrt{\log n}$*. Then, there exist constants* (c_0, c_1, c_2, c_3) *so that for any* $i \in [\mathcal{I}]$ *and* $t \in [t_{i-1}, t_i]$ *with* $1 < \frac{t_i}{t_{i-1}} \le 2$*,*

1. *Denote* $\operatorname{dist}(w, [-1,1]^{D_Y})$ *as the distance of point* $w \in \mathbb{R}^{D_Y}$ *to set* $[-1,1]^{D_Y}$*. Then for any* $x \in [-1,1]^{D_X}$*,*

$$\begin{aligned}
&\int_{\mathbb{R}^{D_Y}} \left\|\nabla \log p_{t|x}(w) - S(w, x, t)\right\|^2 p_{t|x}(w)\,\mathrm{d}w \\
\le &\int_{\mathbb{R}^{D_Y}} \left\|\nabla \log p_{t|x}(w) - S(w, x, t)\right\|^2 p_{t|x}(w) \cdot \mathbb{1}\left(\operatorname{dist}(w, [-1,1]^{D_Y}) \le c_0 \sigma_{t_{i-1}}\sqrt{\log n}\right)\,\mathrm{d}w \\
&\qquad + (1 + c^2) \cdot c_1 \frac{1}{n^2}.
\end{aligned}$$

2. *For any* $x \in [-1,1]^{D_X}$ *and* $w \in \mathbb{R}^{D_Y}$ *satisfying* $\operatorname{dist}(w, [-1,1]^{D_Y}) \le c_0 \sigma_{t_{i-1}}\sqrt{\log n}$*, we have*
   (a) $\|\nabla \log p_{t|x}(w)\|_\infty \le c_2 \frac{\sqrt{\log n}}{\sigma_{t_{i-1}}}$*.*
   (b) $(2\pi\sigma_t^2)^{\frac{D}{2}} p_{t|x}(w) \ge n^{-c_3}$*.*

The proof of Lemma D.2 directly follows from Lemma A.2-A.4 of [2]. Then we fix a time interval $t \in [\underline{t}, \bar{t}]$ where $1 < \frac{\bar{t}}{\underline{t}} \le 2$. Then similar as lemma C.6, we demonstrate that it is enough to provide local approximations to the score function.

Lemma D.3. *Suppose $\tau \le \underline{t} \le T$, $\varepsilon_2 > 0$, and $\varepsilon_1 \ge \sigma_{\underline{t}}\sqrt{\log n}$. Let $\mathcal{N}^X_{\varepsilon_2} = (\widetilde{x}_1, \widetilde{x}_2, \cdots, \widetilde{x}_{J_2})$ be one of the largest ε_2-packing of $[-1,1]^{D_X}$, and let $\mathcal{N}^Y_{\varepsilon_1} = (\widetilde{y}_1, \widetilde{y}_2, \cdots, \widetilde{y}_{J_1})$ be one of the largest ε_1-packing of $[-1,1]^{D_Y}$. Then if for any $j_1 \in [J_1]$ and $j_2 \in [J_2]$, there exists a neural network $\phi^*_{j_1 j_2}(x,w,t) \in \Phi\big(H, W, R, B, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ so that for any $t \in [\underline{t}, \overline{t}]$, $x \in \mathbb{B}_{[-1,1]^{D_X}}(\widetilde{x}_{j_2}, \sqrt{2}\varepsilon_2)$ and $w \in \mathbb{R}^{D_Y}$ satisfying $\|w - \widetilde{y}_{j_1}\| \le \sqrt{2}(2\varepsilon_1 + c_0\sigma_{\underline{t}}\sqrt{\log n})$ and $\mathrm{dist}(w, [-1,1]^{D_X}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}$,*

$$\|\phi^*_{j_1 j_2}(w,x,t) - \nabla \log p_{t|x}(w)\|_\infty \le \varepsilon.$$

Then there exists a neural network $\phi_{\mathrm{score}}(w,x,t) \in \big(H_1, W_1, R_1, B_1, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ with $H_1 = \Theta(H + \log^2 n)$, $\|W_1\|_\infty = \Theta(J_1 J_2(\|W\|_\infty + \log n) + \log^3 n)$, $R_1 = \Theta(J_1 J_2 (R + \log n) + \log^4 n)$ and $B_1 = \exp(\Theta(\log^2 n)) \vee B$, so that for any $t \in [\underline{t}, \overline{t}]$, $x \in [-1,1]^{D_X}$ and $w \in \mathbb{R}^{D_Y}$ satisfying $\mathrm{dist}(x, [-1,1]^{D_Y}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}$,

$$\|\phi_{\mathrm{score}}(w,x,t) - \nabla \log p_{t|x}(w)\|_\infty \lesssim \varepsilon + \frac{1}{n}.$$

The proof of Lemma D.3 can be conducted similarly to the proof of Lemma C.6. Then similar as (2), by statement 2 of Lemma D.2, there exists a large enough constant c_2, so that for any $t \in [\underline{t}, \overline{t}]$, $x \in [-1,1]^{D_X}$, $w \in \mathbb{R}^{D_Y}$ with $\mathrm{dist}(w, [-1,1]^{D_Y}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}$, and any partition $\{\mathcal{A}_{(x,w)}, [-1,1]^{D_Y} \backslash \mathcal{A}_{(x,w)}\}$ of $[-1,1]^{D_Y}$ satisfying $\{y \in [-1,1]^{D_Y} : \|y - w\| \le c_2\sigma_{\underline{t}}\sqrt{\log n}\} \subset \mathcal{A}_{w,x}$, it holds that

$$\left\| \nabla \log p_{t|x}(w) - \frac{1}{\sigma_t} \cdot \frac{\mathbb{E}_{y\sim\mu^*_{Y|x}}\Big[\exp\Big(-\frac{\|w - m_t y\|^2}{2\sigma_t^2}\Big) \cdot -\frac{(w - m_t y)}{\sigma_t} \mathbf{1}(y \in \mathcal{A}_{(x,w)})\Big]}{\mathbb{E}_{y\sim\mu^*_{Y|x}}\Big[\exp\Big(-\frac{\|w - m_t y\|^2}{2\sigma_t^2}\Big) \mathbf{1}(y \in \mathcal{A}_{(x,w)})\Big]} \right\|_\infty \le \frac{1}{n}. \tag{32}$$

We will approximate $\nabla \log p_{t|x}(w)$ by constructing suitable sets $\mathcal{A}_{(x,w)}$ for small $\underline{t}$ and large $\underline{t}$.

D.1.1 Case 1: $n^{-\frac{2}{2\alpha_Y + D_Y + D_X\frac{\alpha_Y}{\alpha_X}}} \le \underline{t} \le T$

Set $\varepsilon_1 = \sigma_{\underline{t}}\sqrt{\log n}$, $\varepsilon_2 = n^{-\frac{1}{2\alpha_X + D_X}}(\sigma_{\underline{t}}\sqrt{\log n})^{-\frac{D_Y}{2\alpha_X + D_X}}$. Let $\mathcal{N}^X_{\varepsilon_2}$ be one of the largest ε_2-packing of $[-1,1]^{D_X}$ and $\mathcal{N}^Y_{\varepsilon_1}$ be one of the largest ε_1-packing of $[-1,1]^{D_Y}$. Then we have $J_1 = |\mathcal{N}^Y_{\varepsilon_1}| \lesssim \varepsilon_1^{-D_Y}$ and $J_2 = |\mathcal{N}^X_{\varepsilon_2}| \lesssim \varepsilon_2^{-D_X}$. Now we take an arbitrary $\widetilde{x} \in \mathcal{N}^X_{\varepsilon_2}$ and $\widetilde{y} \in N^Y_{\varepsilon_1}$, consider set

$$\begin{aligned}\mathscr{S}_{\widetilde{x}\widetilde{y}} = \Big\{&(x,w) : x \in \mathbb{B}_{[-1,1]^{D_X}}(\widetilde{x}, \sqrt{2}\varepsilon_2),\\ &\|w - \widetilde{y}\| \le c_3\,\sigma_{\underline{t}}\sqrt{\log n}, \mathrm{dist}(w, [-1,1]^{D_Y}) \le c_0\sigma_{\underline{t}}\sqrt{\log n}\Big\},\end{aligned}$$

we claim that

Claim 5. *There exists $\phi^*(w,x,t) \in \Phi\big(H, W, R, B, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \widetilde{\Theta}(1)$, $R = \widetilde{\Theta}(1)$, $B = \exp(\Theta(\log^4 n))$, so that for any $(x,w) \in \mathscr{S}_{\widetilde{x}\widetilde{y}}$, and $t \in [\underline{t}, \overline{t}]$,*

$$\|\phi^*(w,x,t) - \nabla \log p_{t|x}(w)\|_\infty = \widetilde{\mathcal{O}}\Big(\frac{\varepsilon_2^{\alpha_X}}{\sigma_{\underline{t}}}\Big).$$

Then the second statement of Lemma D.1 directly follows from Lemmas D.2 and D.3. Now we show Claim 5.

Firstly, notice that for any $(x,w) \in \mathscr{S}_{\widetilde{x}\widetilde{y}}$,

$$\begin{aligned}&\{y \in [-1,1]^{D_Y} : \|y - w\| \le c_2\sigma_{\underline{t}}\sqrt{\log n}\}\\ &\subset \{y \in [-1,1]^{D_Y} : \|y - \widetilde{y}\| \le c_2\sigma_{\underline{t}}\sqrt{\log n} + \|w - \widetilde{y}\|\}\\ &\subset \{y \in [-1,1]^{D_Y} : \|y - \widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}\}.\end{aligned}$$

Therefore, by equation (32), we only need to approximate

$$\frac{1}{\sigma_t} \cdot \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y}. \tag{33}$$

Let

$$\mu^*|_{\widetilde{x}}(y|x) = \sum_{\substack{j \in \mathbb{N}_0^{d_X} \\ |j| < \alpha_X}} \frac{\mu^*{}_{(0,j)}(y|\widetilde{x})}{j!}(x-\widetilde{x})^j.$$

Then when $y \in [-1,1]^{D_Y}$ and $x \in [-1,1]^{D_X}$,

$$|\mu^*(y|x) - \mu^*|_{\widetilde{x}}(y|x)| \lesssim \|x-\widetilde{x}\|^{\alpha_X} \lesssim \varepsilon_2^{\alpha_X}.$$

So we have

$$\begin{aligned}
&\Bigg\| \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \\
&\quad - \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y} \Bigg\| \\
&\le \Bigg\| \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \\
&\qquad - \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \Bigg\| \\
&\qquad + \Bigg\| \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \\
&\qquad\quad - \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y} \Bigg\| \\
&\lesssim \sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}}} \left(\left\| \frac{w-m_t y}{\sigma_t} \right\| \cdot \frac{|\mu^*(y|x) - \mu^*|_{\widetilde{x}}(y|x)|}{\mu^*(y|x)} \right) \\
&+ \Bigg\| \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \Bigg\| \\
&\qquad \cdot \Bigg\| \frac{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) (\mu^*|_{\widetilde{x}}(y|x) - \mu^*(y|x))\,\mathrm{d}y}{\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y} \Bigg\| \\
&\lesssim \sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}}} \left(\left\| \frac{w-m_t y}{\sigma_t} \right\| \cdot \frac{|\mu^*(y|x) - \mu^*|_{\widetilde{x}}(y|x)|}{\mu^*(y|x)} \right) \\
&\qquad + \sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}}} \left\| \frac{w-m_t y}{\sigma_t} \right\| \cdot \sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}}} \frac{|\mu^*(y|x) - \mu^*|_{\widetilde{x}}(y|x)|}{\mu^*|_{\widetilde{x}}(y|x)} \\
&\lesssim \sqrt{\log n} \cdot \varepsilon_2^{\alpha_X},
\end{aligned}$$

where the last inequality uses the lower boundedness of $\mu^*(y|x)$ over $y \in [-1,1]^{D_Y}$. Then notice that for any $(x,w) \in \mathscr{S}_{\widetilde{x}\widetilde{y}}$ and $\|y-\widetilde{y}\| \lesssim \sigma_{\underline{t}}\sqrt{\log n}$,

$$\|w - m_t y\| \le \|w - \widetilde{y}\| + \|\widetilde{y} - y\| + \|y - m_t y\| \le C\,\sigma_{\underline{t}}\sqrt{\log n}. \tag{34}$$

Therefore, denote

$$\overline{dp}_t(w,x) = \int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y,$$

and

$$\overline{p}_t(w,x) = \int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y.$$

We can derive

$$\left\|\frac{\overline{dp}_t(w,x)}{\overline{p}_t(w,x)}\right\| \lesssim \sqrt{\log n},$$

and

$$\overline{p}_t(w,x) \gtrsim n^{-C}\sigma_{\underline{t}}^{D_Y}.$$

Therefore, if there exist neural networks $\phi^{[1]}(w,x,t)$ and $\phi^{[2]}(w,x,t)$ so that for any $t \in [\underline{t},\overline{t}]$ and $(x,w) \in \mathscr{S}_{\widetilde{x}\widetilde{y}}$,

$$\|\overline{dp}_t(w,x) - \phi^{[1]}(w,x,t)\|_\infty = \widetilde{\mathcal{O}}\left((\sigma_{\underline{t}})^{D_Y}\varepsilon_2^{\alpha_X} n^{-C}\right), \tag{35}$$

$$\|\overline{p}_t(w,x) - \phi^{[2]}(w,x,t)\|_\infty = \widetilde{\mathcal{O}}\left((\sigma_{\underline{t}})^{D_Y}\varepsilon_2^{\alpha_X} n^{-C}\right). \tag{36}$$

Then we have

$$\left\|\frac{1}{\sigma_t}\cdot\frac{\overline{dp}_t(x)}{\overline{p}_t(x)} - \frac{1}{\sigma_t}\cdot\frac{\phi^{[1]}(x,t)}{\phi^{[2]}(x,t)}\right\|_\infty = \widetilde{\mathcal{O}}\left(\frac{\varepsilon_2^{\alpha_X}}{\sigma_{\underline{t}}}\right). \tag{37}$$

To construct $\phi^{[1]}(w,x,t)$, use (34), by choosing $\mathscr{L} = \Theta(\log n)$, we have

$$\left|\exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) - \sum_{l_1=0}^{\mathscr{L}}(-1)^{l_1}\frac{\|w-m_t y\|^{2l_1}}{2^{l_1}l_1!\sigma_t^{2l_1}}\right| \lesssim n^{-2-C}.$$

Therefore, we have

$$\left\|\overline{dp}_t(w,x) - \int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \sum_{l_1=0}^{\mathscr{L}}(-1)^{l_1}\frac{\|w-m_t y\|^{2l_1}}{2^{l_1}l_1!\sigma_t^{2l_1}} \cdot \left(-\frac{w-m_t y}{\sigma_t}\right)\mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y\right\| \lesssim (\sigma_t)^{D_Y} n^{-1-C}. \tag{38}$$

Then notice that $\mu^*|_{\widetilde{x}}(y|x)$ is polynomial in x,

$$\int_{\|y-\widetilde{y}\|_\infty \le c_4\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \sum_{l_1=0}^{\mathscr{L}}(-1)^{l_1}\frac{\|w-m_t y\|^{2l_1}}{2^{l_1}l_1!\sigma_t^{2l_1}} \cdot \left(-\frac{w-m_t y}{\sigma_t}\right)\mu^*|_{\widetilde{x}}(y|x)\,\mathrm{d}y$$
$$= \sum_{l_1=0}^{\mathscr{L}}\left(\frac{1}{\sigma_t}\right)^{2l_1+1} \sum_{0\le k\le 2l_1+1} m_t^k \sum_{i\in\mathbb{N}_0^{D_Y}, |i|\le 2l_1+1} w^{(i)} \sum_{j\in\mathbb{N}_0^{D_X}, |j|\le\lfloor\alpha_X\rfloor} a_{l_1kij}x^{(j)},$$

where $a_{l_1kij} \in \mathbb{R}^{D_Y}$ are some constant coefficients. So similar as the analysis for the manifold setting, there exists networks $\phi^{[1]}(w,x,t) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \widetilde{\Theta}(1)$, $R = \widetilde{\Theta}(1)$, $B = \exp(\Theta(\log^4 n))$ so that (35) holds. Similarly, there exists a neural network $\phi^{[2]}(x,t)$ with the same size as $\phi^{[1]}(x,t)$ so that (36) holds. Then using (37) and Lemmas C.7-C.10, we can obtain Claim 5.

D.1.2 Case 2: $\tau \leq \underline{t} \leq n^{-\frac{2}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}}$

We set $\varepsilon_1 = n^{-\frac{1}{2\alpha_Y + d_Y + d_X \frac{\alpha_Y}{\alpha_X}}}$ and $\varepsilon_2 = n^{-\frac{1}{2\alpha_X + d_X + d_Y \frac{\alpha_X}{\alpha_Y}}}$. Let $\mathcal{N}^X_{\varepsilon_2}$ be one of the largest ε_2-packing of $[-1,1]^{D_X}$ and $\mathcal{N}^Y_{\varepsilon_1}$ be one of the largest ε_1-packing of $[-1,1]^{D_X}$. Then we have $J_1 = |\mathcal{N}^Y_{\varepsilon_1}| \lesssim \varepsilon_1^{-d_Y}$ and $J_2 = |\mathcal{N}^X_{\varepsilon_2}| \lesssim \varepsilon_2^{-d_X}$. Then take an arbitrary $\widetilde{x} \in \mathcal{N}^X_{\varepsilon_2}$ and $\widetilde{y} \in N^Y_{\varepsilon_1}$, Consider set

$$
\begin{aligned}
\mathscr{S}_{\widetilde{x}\widetilde{z}} = \Big\{ &(x, w) \,:\, x \in \mathbb{B}_{[-1,1]^{D_X}}(\widetilde{x}, \sqrt{2}\varepsilon_2), \\
&\|w - \widetilde{y}\| \leq C\,\varepsilon_1, \mathrm{dist}(w, [-1,1]^{D_Y}) \leq c_0 \sigma_{\underline{t}} \sqrt{\log n} \},
\end{aligned}
$$

we claim that

Claim 6. *There exists $\phi^*(w, x, t) \in \Phi\big(H, W, R, B, \Theta(\frac{\sqrt{\log n}}{\sigma_{\underline{t}}})\big)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \widetilde{\Theta}(1)$, $R = \widetilde{\Theta}(1)$, $B = \exp(\Theta(\log^4 n))$, so that for any $(x, w) \in \mathscr{S}_{\widetilde{x}\widetilde{y}}$, and $t \in [\underline{t}, \overline{t}]$,*

$$
\|\phi^*(w, x, t) - \nabla \log p_{t|x}(w)\|_\infty = \widetilde{\mathcal{O}}\Big(\frac{\varepsilon_1^{\alpha_Y}}{\sigma_{\underline{t}}}\Big).
$$

Then the desired result directly follows from Lemmas D.2 and D.3. Now we show Claim 6. For any $(x, w) \in \mathscr{S}_{\widetilde{x}\widetilde{y}}$, we have

$$
\{y \in [-1,1]^{D_Y} \,:\, \|y - w\| \leq c_2 \sigma_{\underline{t}} \sqrt{\log n}\} \subset \{y \in [-1,1]^{D_Y} \,:\, \|y - w\|_\infty \leq c_2 \sigma_{\underline{t}} \sqrt{\log n}\}.
$$

Moreover, notice that μ^* is C^{α_Y, α_X}-smooth, we can write

$$
\mu^*|_{(\widetilde{y}, \widetilde{x})}(y|x) = \sum_{(j_1, j_2) \in \mathcal{J}^{D_Y, D_X}_{\alpha_Y, \alpha_X}} \frac{\mu^*{}_{(j_1, j_2)}(\widetilde{y}, \widetilde{x})}{j_1! j_2!} (y - \widetilde{y})^{j_1} (x - \widetilde{x})^{j_2}, \tag{39}
$$

where for any $x \in [-1,1]^{D_X}$ and $y \in [-1,1]^{D_Y}$,

$$
\|\mu^*|_{(\widetilde{y}, \widetilde{x})}(y|x) - \mu^*(y, x)\| \lesssim \|y - \widetilde{y}\|^{\alpha_Y} + \|x - \widetilde{x}\|^{\alpha_X}.
$$

So we have

$$
\begin{aligned}
&\left\| \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \right. \\
&\left. - \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)\,\mathrm{d}y} \right\| \\
\le &\left\| \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \right. \\
&\qquad \left. - \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \right\| \\
&\qquad + \left\| \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \right. \\
&\qquad\qquad \left. - \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)\,\mathrm{d}y} \right\| \\
\lesssim &\sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}}} \left(\left\| \frac{w-m_t y}{\sigma_t} \right\| \cdot \frac{|\mu^*(y|x) - \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)|}{\mu^*(y|x)} \right) \\
+ &\left\| \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \cdot \left(-\frac{w-m_t y}{\sigma_t}\right) \mu^*(y|x)\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*(y|x)\,\mathrm{d}y} \right\| \\
&\qquad \cdot \left\| \frac{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) (\mu^*|_{(\widetilde{y},\widetilde{x})}(y|x) - \mu^*(y|x))\,\mathrm{d}y}{\int_{\|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}} \mathbf{1}(y \in [-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right) \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)\,\mathrm{d}y} \right\| \\
\lesssim &\sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}}} \left(\left\| \frac{w-m_t y}{\sigma_t} \right\| \cdot \frac{|\mu^*(y|x) - \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)|}{\mu^*(y|x)} \right) \\
&\quad + \sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}}} \left\| \frac{w-m_t y}{\sigma_t} \right\| \cdot \sup_{\substack{y \in [-1,1]^{D_X} \\ \|y-w\|_\infty \le c_2 \sigma_{\underline{t}} \sqrt{\log n}}} \frac{|\mu^*(y|x) - \mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)|}{\mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)} \\
\lesssim &\sqrt{\log n} \cdot \varepsilon_1^{\alpha_Y}.
\end{aligned} \tag{40}
$$

For any $s \in [D_Y]$, denote $\mathbf{1}^s = (\mathbf{1}_1^s, \mathbf{1}_2^s, \cdots, \mathbf{1}_{D_Y}^s)$ as the D_Y-dimensional vector where the sth element being 1 and other elements being 0 (i.e., $\mathbf{1}_k^s = \mathbf{1}(s=k)$), and denote

$$
\begin{aligned}
&\widetilde{dp}_{ts}(w,x)\\
&= \int_{\|y-w\|_\infty \le c_2\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y\in[-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\cdot\left(-\frac{w_s-m_t y_s}{\sigma_t}\right)\mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)\,\mathrm{d}y\\
&= -\frac{1}{\sigma_t}\cdot \sum_{(j_1,j_2)\in\mathcal{J}_{\alpha_Y,\alpha_X}^{D_Y,D_X}} \frac{\mu^*{}_{(j_1,j_2)}(\widetilde{y},\widetilde{x})}{j_1!j_2!}(x-\widetilde{x})^{j_2}\\
&\quad \cdot \int_{\|y-w\|_\infty \le c_2\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y\in[-1,1]^{D_X}) \prod_{s_1=1}^{D_Y} \exp\Big(-\frac{(w_{s_1}-m_t y_{s_1})^2}{2\sigma_t^2}\Big)(w_{s_1}-m_t y_{s_1})^{\mathbf{1}_{s_1}^s}(y_{s_1}-\widetilde{y}_{s_1})^{j_{1s_1}}\,\mathrm{d}y\\
&= -\frac{1}{\sigma_t}\cdot \sum_{(j_1,j_2)\in\mathcal{J}_{\alpha_Y,\alpha_X}^{D_Y,D_X}} \frac{\mu^*{}_{(j_1,j_2)}(\widetilde{y},\widetilde{x})}{j_1!j_2!}(x-\widetilde{x})^{j_2}\\
&\quad \cdot \prod_{s_1=1}^{D_Y} \int_{-1\vee(w_{s_1}-c_2\sigma_{\underline{t}}\sqrt{\log n})}^{1\wedge(w_{s_1}+c_2\sigma_{\underline{t}}\sqrt{\log n})} \exp\Big(-\frac{(w_{s_1}-m_t y_{s_1})^2}{2\sigma_t^2}\Big)(w_{s_1}-m_t y_{s_1})^{\mathbf{1}_{s_1}^s}(y_{s_1}-\widetilde{y}_{s_1})^{j_{1s_1}}\,\mathrm{d}y_{s_1},
\end{aligned}
$$

and

$$
\begin{aligned}
\widetilde{p}_t(w,x) &= \int_{\|y-w\|_\infty \le c_2\sigma_{\underline{t}}\sqrt{\log n}} \mathbf{1}(y\in[-1,1]^{D_X}) \exp\left(-\frac{\|w-m_t y\|^2}{2\sigma_t^2}\right)\mu^*|_{(\widetilde{y},\widetilde{x})}(y|x)\,\mathrm{d}y\\
&= \sum_{(j_1,j_2)\in\mathcal{J}_{\alpha_Y,\alpha_X}^{D_Y,D_X}} \frac{\mu^*{}_{(j_1,j_2)}(\widetilde{y},\widetilde{x})}{j_1!j_2!}(x-\widetilde{x})^{j_2}\cdot \prod_{s_1=1}^{D_Y} \int_{-1\vee(w_{s_1}-c_2\sigma_{\underline{t}}\sqrt{\log n})}^{1\wedge(w_{s_1}+c_2\sigma_{\underline{t}}\sqrt{\log n})} \exp\Big(-\frac{(w_{s_1}-m_t y_{s_1})^2}{2\sigma_t^2}\Big)(y_{s_1}-\widetilde{y}_{s_1})^{j_{1s_1}}\,\mathrm{d}y_{s_1}.
\end{aligned}
$$

Then notice that for any $(x,w)\in\mathscr{S}_{\widetilde{x}\widetilde{y}}$, and any $y\in[-1,1]^{D_Y}$ satisfying $\|y-w\|_\infty \le c_2\sigma_{\underline{t}}\sqrt{\log n}$:

$$\|w-m_t y\| \le \|w-y\| + \|y-m_t y\| \le C\,\sigma_{\underline{t}}\sqrt{\log n},$$

we can derive

$$\left\|\frac{\widetilde{dp}_t(w,x)}{\widetilde{p}_t(w,x)}\right\| \lesssim \sqrt{\log n},$$

and

$$\widetilde{p}_t(w,x) \gtrsim n^{-C}(\sigma_{\underline{t}})^{D_Y}.$$

Therefore, if there exist neural networks $\phi^{[1]}(w,x,t)$ and $\phi^{[2]}(w,x,t)$ so that for any $t\in[\underline{t},\overline{t}]$ and $(x,w)\in\mathscr{S}_{\widetilde{x}\widetilde{y}}$,

$$\|\widetilde{dp}_t(w,x) - \phi^{[1]}(w,x,t)\|_\infty = \widetilde{\mathcal{O}}\left((\sigma_{\underline{t}})^{D_Y}\left(\varepsilon_1^{\alpha_Y}\right)n^{-C}\right), \tag{41}$$

$$\|\widetilde{p}_t(w,x) - \phi^{[2]}(w,x,t)\|_\infty = \widetilde{\mathcal{O}}\left((\sigma_{\underline{t}})^{D_Y}\varepsilon_1^{\alpha_Y}n^{-C}\right). \tag{42}$$

Then we have

$$\left\|\frac{1}{\sigma_t}\cdot\frac{\widetilde{dp}_t(x)}{\widetilde{p}_t(x)} - \frac{1}{\sigma_t}\cdot\frac{\phi^{[1]}(x,t)}{\phi^{[2]}(x,t)}\right\|_\infty = \widetilde{\mathcal{O}}\left(\frac{\varepsilon_2^{\alpha_X}+\varepsilon_1^{\alpha_Y}}{\sigma_{\underline{t}}}\right). \tag{43}$$

Then we construct $\phi^{[1]}(w,x,t)$ by approximating $\widetilde{dp}_t(w,x)$ with polynomials. By choosing $\mathscr{L} = \Theta(\log n)$, we have for any $s_1\in[D_Y]$,

$$\left|\exp\left(-\frac{(w_{s_1}-m_t y_{s_1})^2}{2\sigma_t^2}\right) - \sum_{l_1=0}^{\mathscr{L}}(-1)^{l_1}\frac{(w_{s_1}-m_t y_{s_1})^{2l_1}}{2^{l_1}l_1!\sigma_t^{2l_1}}\right| \lesssim n^{-2-C}.$$

Then for any $s \in [D_Y]$, we can write

$$
\begin{aligned}
&-\frac{1}{\sigma_t} \cdot \sum_{(j_1,j_2)\in \mathcal{J}_{\alpha_Y,\alpha_X}^{D_Y,D_X}} \frac{\mu^*{}_{(j_1,j_2)}(\widetilde{y},\widetilde{x})}{j_1! j_2!}(x-\widetilde{x})^{j_2} \\
&\quad \cdot \prod_{s_1=1}^{D_Y} \int_{-1\vee(w_{s_1}-c_2\sigma_{\underline{t}}\sqrt{\log n})}^{1\wedge(w_{s_1}+c_2\sigma_{\underline{t}}\sqrt{\log n})} \sum_{l_1=0}^{\mathscr{L}} (-1)^{l_1} \frac{(w_{s_1}-m_t y_{s_1})^{2l_1}}{2^{l_1} l_1! \sigma_t^{2l_1}} (w_{s_1}-m_t y_{s_1})^{\mathbf{1}_{s_1}^s} (y_{s_1}-\widetilde{y}_{s_1})^{j_{1s_1}}\, \mathrm{d}y_{s_1} \\
&= -\frac{1}{\sigma_t} \cdot \sum_{(j_1,j_2)\in \mathcal{J}_{\alpha_Y,\alpha_X}^{D_Y,D_X}} \frac{\mu^*{}_{(j_1,j_2)}(\widetilde{y},\widetilde{x})}{j_1! j_2!}(x-\widetilde{x})^{j_2} \\
&\quad \cdot \prod_{s_1=1}^{D_Y} \sum_{l_1=0}^{\mathscr{L}_1} (\frac{1}{\sigma_t})^{2l_1} \sum_{0\le k\le 2l_1+1} m_t^k \\
&\sum_{0\le s_2\le 2+j_{1s_1}} (-1\vee(w_{s_1}-c_2\sigma_{\underline{t}}\sqrt{\log n}))^{s_2} \sum_{0\le s_3\le 2+j_{1s_1}} (1\wedge(w_{s_1}+c_2\sigma_{\underline{t}}\sqrt{\log n}))^{s_3} \sum_{0\le i\le 2l_1+1} a_{sj_1s_1l_1ks_2s_3i} w_{s_1}^i.
\end{aligned}
$$

So similar as the analysis for the manifold setting, there exists networks $\phi^{[1]}(w,x,t) \in \Phi(H,W,R,B)$ with $H = \Theta(\log^4 n)$, $\|W\|_\infty = \widetilde{\Theta}(1)$, $R = \widetilde{\Theta}(1)$, $B = \exp(\Theta(\log^4 n))$ so that (41) holds. Similarly, there exists a neural network $\phi^{[2]}(x,t)$ with the same size as $\phi^{[1]}(x,t)$ so that (42) holds. Then using (40), (43), and Lemmas C.7-C.10, we can obtain Claim 6.

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