

# Nonparametric Estimation of a Factorizable Density using Diffusion Models

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## Abstract

In recent years, diffusion models, and more generally score-based deep generative models, have achieved remarkable success in various applications, including image and audio generation. In this paper, we view diffusion models as an implicit approach to nonparametric density estimation and study them within a statistical framework to analyze their surprising performance. A key challenge in high-dimensional statistical inference is leveraging low-dimensional structures inherent in the data to mitigate the curse of dimensionality. We assume that the underlying density exhibits a low-dimensional structure by factorizing into low-dimensional components, a property common in examples such as Bayesian networks and Markov random fields. Under suitable assumptions, we demonstrate that an implicit density estimator constructed from diffusion models adapts to the factorization structure and achieves the minimax optimal rate with respect to the total variation distance. In constructing the estimator, we design a sparse weight-sharing neural network architecture, where sparsity and weight-sharing are key features of practical architectures such as convolutional neural networks and recurrent neural networks.

**Keywords:** Bayesian network, diffusion model, factorizable density, Markov random field, minimax optimality, score-based generative model, weight-sharing neural network

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## 1. Introduction

Suppose we have observations  $\mathbf{X}^1, \dots, \mathbf{X}^n$ , which are independent and identically distributed  $D$ -dimensional random variables following an unknown distribution  $P_0$  with density  $p_0$ . Inference of the unknown  $P_0$  or its density  $p_0$  is a fundamental task in unsupervised learning, and various methodologies and related theories have been developed over the past few decades (e.g., Hastie et al., 2009; Tsybakov, 2008; Giné and Nickl, 2016).

Among these approaches, *diffusion models* have recently demonstrated remarkable success across a wide range of applications. Even when compared to other modern deep generative models such as variational autoencoders (VAEs) (Kingma and Welling, 2014; Rezende et al., 2014), generative adversarial networks (GANs) (Goodfellow et al., 2014; Arjovsky et al., 2017; Mroueh et al., 2018), and normalizing flows (Dinh et al., 2015; Rezende and Mohamed, 2015), diffusion models have achieved state-of-the-art performance in domains including image (Rombach et al., 2022; Dhariwal and Nichol, 2021), video (Ho et al., 2022), and audio generation (Kong et al., 2021).

Rather than directly estimating  $p_0$ , diffusion models, more generally referred to as score-based generative models, aim to estimate the map  $\mathbf{x} \mapsto \nabla \log p_0(\mathbf{x})$ , commonly known as the score function. They can be regarded as an implicit approach to density estimation because, although no direct estimator of  $p_0$  is constructed, the estimated score function enables sampling from the learned distribution, for example, via score-based Markov chain Monte Carlo algorithms such as Hamiltonian or Langevin Monte Carlo (Neal, 2011). The idea of score-function estimation was first proposed by Hyvärinen (2005) and subsequently extended by Vincent (2011) and Song et al. (2020).

A diffusion model consists of two diffusion processes, namely the forward and the backward/reverse processes. The forward process is typically a simple and well-known diffusion, such as the Ornstein–Uhlenbeck (OU) process, while the drift term in the reverse process involves the score functions corresponding to the marginal densities of the forward process. Rather than estimating a single score function  $\nabla \log p_0(\cdot)$ , diffusion models (Sohl-Dickstein et al., 2015; Ho et al., 2020; Song and Ermon, 2019; Song et al., 2021) jointly estimate the family of score functions; see Section 2 for further details.

For large  $D$ , inferring high-dimensional distributions becomes prohibitively difficult due to the well-known curse of dimensionality. Why, then, do diffusion models perform so well in practice, especially in high-dimensional domains such as images and videos? A natural explanation is that although the ambient dimension  $D$  is large, real-world data often lie on, or near, low-dimensional structures that effectively mitigate this curse. This perspective aligns with a long line of statistical research showing that structural assumptions, such as sparsity (Hastie et al., 2015), additivity (Hastie and Tibshirani, 1990), and manifold structures (Genovese et al., 2012), can substantially improve statistical efficiency. In the presence of such low-dimensional structures, estimators can achieve significantly faster convergence rates even in high-dimensional settings. In practice, however, the underlying structure is typically unknown, and procedures that can adapt to such unknown structures are therefore preferred. Deep neural networks (DNNs), for instance, have been shown to possess remarkable adaptivity in a variety of function estimation problems (Imaizumi and Fukumizu, 2022; Schmidt-Hieber, 2020; Tang and Yang, 2024; Chae et al., 2023).

Motivated by this viewpoint, we focus on a specific low-dimensional structure that captures a broad family of distributions: *factorizable densities*. We assume that the density function  $p_0$  admits the factorization

$$p_0(\mathbf{x}) = \prod_{I \in \mathcal{I}} g_I(\mathbf{x}_I), \quad (1)$$

where  $\mathcal{I} \subseteq 2^{[D]}$  is a collection of index sets,  $\mathbf{x}_I = (x_i)_{i \in I}$ , and each  $g_I$  is a  $|I|$ -variate function. Here,  $[D] = \{1, \dots, D\}$  and  $|I|$  denotes the cardinality of  $I$ . Such factorizable densities naturally arise in graphical model contexts (Liu and Lafferty, 2019), including Bayesian networks and Markov random fields. In particular, the conditional-independence structures induced by undirected graphical models (Markov random fields) are well suited for modeling images, where spatially adjacent pixels tend to be strongly correlated, whereas distant pixels exhibit weak correlations (Ji, 2020; Vandermeulen et al., 2024b,a); see Section 4 for further details.

Although this structure is well known in the statistical community, nonparametric adaptive procedures for such models have rarely been investigated in the literature. For  $\beta$ -Hölder densities (as defined in Section 1.1), classical nonparametric theory suggests that incorporating a factorization structure can improve the convergence rate with respect to the total variation distance, from  $n^{-\beta/(D+2\beta)}$  (Tsybakov, 2008; Giné and Nickl, 2016) to  $n^{-\beta/(d+2\beta)}$ , where  $d = \max_{I \in \mathcal{I}} |I|$  denotes the effective dimension corresponding to the largest component function. Here, we assume that  $D$  is fixed and that all component functions have the same smoothness level  $\beta$ .

Once the factorization form in (1) is known, it is not difficult to construct an estimator for  $p_0$  that achieves the rate  $n^{-\beta/(d+2\beta)}$  under suitable technical conditions. It remains challenging, however, to construct an estimator that adapts to the unknown factorization structure. To the best of our knowledge, theoretically adaptive estimators (though not necessarily achieving the optimal rate) have been considered only in a few recent works (Bos and Schmidt-Hieber, 2024; Vandermeulen et al., 2024b,a).

In this paper, we show that the implicit density estimator derived from diffusion models is adaptive to the underlying factorization structure and achieves the minimax-optimal convergence rate for estimating  $\beta$ -Hölder factorizable densities, up to logarithmic factors (Theorem 3). The main theoretical challenge lies in approximating the joint score functions, which are the score functions associated with the marginal densities of the forward diffusion process, using neural networks, since these functions are defined through  $D$ -dimensional integrals. While prior theoretical works (Oko et al., 2023; Tang and Yang, 2024) are based on vanilla sparse neural networks, we employ a novel architecture: *sparse weight-sharing neural networks*. Here, parameters are sparse and shared within each layer to reduce model complexity.

Although sparse weight-sharing neural networks are relatively new in statistical theory, widely used architectures such as convolutional neural networks (CNNs; LeCun et al., 1989; Krizhevsky et al., 2012) and recurrent neural networks (Rumelhart et al., 1986; Sutskever et al., 2014) can be regarded as representative examples. From a theoretical perspective, to the best of our knowledge, only a few works have established that CNNs perform as well as vanilla feedforward networks in terms of approximation or estimation rates (Petersen and Voigtlaender, 2020; Oono and Suzuki, 2019; Yang et al., 2024; Fang and Cheng, 2023).

While finalizing the revision of this article, we became aware of a very recent preprint by Fan et al. (2025), which investigates essentially the same problem, namely, the same estimator, the same structural assumption, and the same convergence result. The key difference lies in the network architecture: they employ fully connected neural networks. Given this finding, our results do not demonstrate a distinct theoretical advantage of sparse weight-sharing neural networks. Nevertheless, based on our proof techniques, it is plausible to conjecture that sparse weight-sharing architectures may approximate certain general classes of functions more efficiently than fully connected ones. We believe that exploring this theoretically intriguing problem would provide valuable insights into the distinct benefits of sparse weight-sharing networks.

Before concluding the introduction, it is worthwhile to review recent advances in the statistical theory of diffusion models. Oko et al. (2023) proved that the implicit density estimator from the diffusion model is minimax optimal within the nonparametric smooth density estimation framework, using total variation and Wasserstein distances as evaluation metrics. Subsequently, Zhang et al. (2024) and Wibisono et al. (2024) relaxed certain technical assumptions in Oko et al. (2023). Although these papers introduced several interesting mathematical techniques for handling diffusion models, they did not address the issue of the curse of dimensionality. To tackle this issue, Tang and Yang (2024) demonstrated that the estimator from the diffusion model is minimax optimal with respect to the Wasserstein metric under the smooth manifold assumption. Under a similar regime, Azangulov et al. (2024) established tighter upper bounds for the convergence rate in terms of the ambient dimension  $D$ . While the manifold structure is an interesting low-dimensional structure, an optimal estimator adaptive to this structure can also be constructed using methods other than diffusion models (Tang and Yang, 2023; Stéphanovitch et al., 2024). Diffusion models have also been analyzed under other low-dimensional structures beyond manifolds (Chen et al., 2023a; Wang et al., 2024; Yakovlev and Puchkin, 2025). Although minimax optimality is not guaranteed in these settings, they commonly assume that  $P_0$  is singular with respect to the  $D$ -dimensional Lebesgue measure, with additional structural constraints.

In particular, while various interesting statistical theories have been developed for VAEs (Kwon and Chae, 2024; Chae et al., 2023) and GANs (Liang, 2021; Uppal et al., 2019; Chae, 2022; Stéphanovitch et al., 2024; Tang and Yang, 2023; Puchkin et al., 2024), the factorization structure (1), which is closely related to the conditional independence structure of directed and undirected graphs, has not been explored in the literature on deep generative models. While the estimators proposed in Bos and Schmidt-Hieber (2024), Vandermeulen et al. (2024a), and Vandermeulen et al. (2024b) are adaptive to the factorization structure, diffusion models can adapt not only to this structure but also to other structures discussed above, making them significantly more practical alternatives.

The remainder of this paper is organized as follows. In Section 2, we introduce diffusion models and define our implicit density estimator. Section 3 presents the class of sparse weight-sharing networks, while Section 4 details the main assumption: the factorization assumption. Our main theoretical results are provided in Section 5. In Section 6, we discuss the benefits of diffusion models compared to the vanilla score matching estimator. We present small experimental results in Section 7 and conclude with discussions in Section 8. All proofs are provided in the Appendix.

### 1.1 Notations and Definitions

Vectors are denoted using boldface notation. For a multi-index  $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_D)^\top \in (\mathbb{Z}_{\geq 0})^D$ , denote  $D^\boldsymbol{\gamma}$  the mixed partial derivative operator  $\partial^{\boldsymbol{\gamma}} / \partial x_1^{\gamma_1} \cdots \partial x_D^{\gamma_D}$ , where  $|\boldsymbol{\gamma}| = \sum_{i=1}^D \gamma_i$ . For any  $\beta, K > 0$ , let  $\mathcal{H}_D^{\beta, K}(A)$  be the class of  $\beta$ -Hölder functions, consisting of every real-valued function  $g$  on  $A \subseteq \mathbb{R}^D$  such that

$$\sum_{\boldsymbol{\gamma} \leq \lfloor \beta \rfloor} \sup_{\mathbf{x} \in A} |(D^\boldsymbol{\gamma} g)(\mathbf{x})| + \sum_{\boldsymbol{\gamma} = \lfloor \beta \rfloor} \sup_{\substack{\mathbf{x}, \mathbf{y} \in A \\ \mathbf{x} \neq \mathbf{y}}} \frac{|(D^\boldsymbol{\gamma} g)(\mathbf{x}) - (D^\boldsymbol{\gamma} g)(\mathbf{y})|}{\|\mathbf{x} - \mathbf{y}\|_\infty^{\beta - \lfloor \beta \rfloor}} \leq K,$$

where  $\lfloor \beta \rfloor$  denotes the largest integer strictly smaller than  $\beta$ . We often denote  $\mathcal{H}_D^{\beta, K}(A)$  as  $\mathcal{H}^{\beta, K}(A)$  when the dimension is obvious from the context. For a vector  $\mathbf{x}$ , we denote the  $\ell^p$ -norm,  $1 \leq p \leq \infty$ , and the number of nonzero elements as  $\|\mathbf{x}\|_p$  and  $\|\mathbf{x}\|_0$ , respectively. Let  $\phi_{\sigma, D}$  be the density function of the multivariate normal distribution  $\mathcal{N}(\mathbf{0}_D, \sigma^2 \mathbb{I}_D)$ , where  $\mathbf{0}_D$  and  $\mathbb{I}_D$  are  $D$ -dimensional zero vector and identity matrix, respectively. For simplicity, we often denote  $\phi_{\sigma, D}$  as  $\phi_\sigma$  when the dimension is obvious from the context. For real numbers  $a$  and  $b$ , let  $a \vee b$  and  $a \wedge b$  be the maximum and minimum of  $a$  and  $b$ , respectively. The notation  $a \lesssim b$  means that  $a \leq Cb$ , where  $C > 0$  is a constant not relevant to the main argument. Similarly,  $a \asymp b$  implies that  $a \lesssim b$  and  $b \lesssim a$ . Finally, the notation  $C = C(A_1, \dots, A_n)$  means that the constant  $C$  depends only on  $A_1, \dots, A_n$ .

## 2. Diffusion Models

In this section, we provide a brief introduction to the diffusion model proposed in Song et al. (2021) and define the estimator studied in our main results. Let  $(\mathbf{X}_t)_{t \geq 0}$  be the process satisfying the stochastic differential equation (SDE)

$$d\mathbf{X}_t = -\alpha_t \mathbf{X}_t dt + \sqrt{2\alpha_t} d\mathbf{B}_t, \quad \mathbf{X}_0 \sim P_0, \quad (2)$$

where  $(\mathbf{B}_t)_{t \geq 0}$  is a standard  $D$ -dimensional Brownian motion and  $t \mapsto \alpha_t : [0, \infty) \rightarrow [0, \infty)$  is a (known) Borel measurable function. The stochastic process  $(\mathbf{X}_t)$  is often referred to as a time-inhomogeneous OU process, and has been studied in Song et al. (2021) and Chen et al. (2023c). For the OU process (2), the transition kernel is explicitly given as Gaussian. Specifically, the conditional distribution of  $\mathbf{X}_t$  given  $\mathbf{X}_0 = \mathbf{x}_0$  is  $\mathcal{N}(\mu_t \mathbf{x}_0, \sigma_t^2 \mathbb{I}_D)$ , where  $\mu_t = \exp(-\int_0^t \alpha_s ds)$  and  $\sigma_t^2 = 1 - \mu_t^2$ . We denote this conditional distribution and the corresponding density as  $P_t(\cdot | \mathbf{x}_0)$  and  $p_t(\cdot | \mathbf{x}_0)$ , respectively. We also denote  $P_t$  and  $p_t$  as the marginal distribution and density of  $\mathbf{X}_t$ , respectively. Hence, we have

$$p_t(\mathbf{x}) = \int \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) dP_0(\mathbf{y}) = \int \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) p_0(\mathbf{y}) d\mathbf{y}.$$

Note that  $p_t$  converges very quickly to the standard Gaussian density as  $t \rightarrow \infty$ ; see Bakry et al. (2014) for a rigorous statement.

Note that the map  $\mathbf{x} \mapsto \mathbf{f}_0(\mathbf{x}, t)$  is the score function corresponding to the marginal density  $p_t$ . As a convention, we also call  $\mathbf{f}_0$  a score function.

For a given non-random  $\bar{T} > 0$ , let  $(\mathbf{Y}_t)_{t \in [0, \bar{T}]}$  be the reverse-time process defined as  $\mathbf{Y}_t = \mathbf{X}_{\bar{T}-t}$ . Then, it is well-known (Anderson, 1982) that  $(\mathbf{Y}_t)_{t \in [0, \bar{T}]}$  is also a diffusion

process under mild assumptions. More specifically, once

$$\int_s^{\bar{T}} \mathbb{E} \left[ p_t(\mathbf{X}_t) + 2\alpha_t \|\nabla \log p_t(\mathbf{X}_t)\|_2^2 \right] dt < \infty \quad \forall s > 0$$

and the map  $t \mapsto \alpha_t$  is bounded from above, we have

$$\begin{aligned} d\mathbf{Y}_t &= [\alpha_{\bar{T}-t} \mathbf{Y}_t + 2\alpha_{\bar{T}-t} \nabla \log p_{\bar{T}-t}(\mathbf{Y}_t)] dt + \sqrt{2\alpha_{\bar{T}-t}} d\mathbf{B}_t \\ &= [\alpha_{\bar{T}-t} \mathbf{Y}_t + 2\alpha_{\bar{T}-t} \mathbf{f}_0(\mathbf{Y}_t, \bar{T} - t)] dt + \sqrt{2\alpha_{\bar{T}-t}} d\mathbf{B}_t, \quad \mathbf{Y}_0 \sim P_{\bar{T}}, \end{aligned} \quad (3)$$

see Theorem 2.1 of Haussmann and Pardoux (1986). Note that the Brownian motions in (2) and (3) are not identical. However, we use the same notation  $\mathbf{B}_t$  to denote a standard Brownian motion as a convention throughout the paper.

Once we have an estimator  $\hat{\mathbf{f}}$  for the score function  $\mathbf{f}_0$ , one can simulate the reverse process starting from a standard Gaussian to obtain samples from the estimated distribution. The score function can be estimated via the score matching (Hyvärinen, 2005) or its scalable variations (Vincent, 2011; Song et al., 2020; Yu et al., 2022).

Let  $\mathcal{F}$  be a class of functions  $(\mathbf{x}, t) \mapsto \mathbf{f}(\mathbf{x}, t)$  used to model the score function  $\mathbf{f}_0$ . A detailed description of the class  $\mathcal{F}$  in our theory is provided in Section 3. At the population level, the best approximator to  $\mathbf{f}_0$  in  $\mathcal{F}$  can be defined as the solution to the following optimization problem

$$\begin{aligned} & \underset{\mathbf{f} \in \mathcal{F}}{\text{minimize}} \int_0^{\bar{T}} \lambda_t \mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t)\|_2^2 \right] dt \\ \iff & \underset{\mathbf{f} \in \mathcal{F}}{\text{minimize}} \int_0^{\bar{T}} \lambda_t \mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \nabla \log p_t(\mathbf{X}_t)\|_2^2 \right] dt, \end{aligned} \quad (4)$$

where  $\lambda_t \geq 0$  is a weight. Based on the well-known fact (Vincent, 2011) that

$$\mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \nabla \log p_t(\mathbf{X}_t)\|_2^2 \right] = \mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \nabla \log p_t(\mathbf{X}_t \mid \mathbf{X}_0)\|_2^2 \right] + C_t, \quad (5)$$

where  $C_t$  is a constant depending only on  $t$  and  $\mathbf{f}_0$  and

$$\nabla \log p_t(\mathbf{x}_t \mid \mathbf{x}_0) = \frac{\partial \log p_t(\mathbf{x}_t \mid \mathbf{x}_0)}{\partial \mathbf{x}_t} = -\frac{\mathbf{x}_t - \mu_t \mathbf{x}_0}{\sigma_t^2},$$

the minimization problem (4) can be equivalently written as

$$\begin{aligned} & \underset{\mathbf{f} \in \mathcal{F}}{\text{minimize}} \int_0^{\bar{T}} \lambda_t \mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \nabla \log p_t(\mathbf{X}_t \mid \mathbf{X}_0)\|_2^2 \right] dt \\ \iff & \underset{\mathbf{f} \in \mathcal{F}}{\text{minimize}} \int_0^{\bar{T}} \lambda_t \mathbb{E} \left[ \mathbb{E} \left( \left\| \mathbf{f}(\mathbf{X}_t, t) + \frac{\mathbf{X}_t - \mu_t \mathbf{X}_0}{\sigma_t^2} \right\|_2^2 \mid \mathbf{X}_0 \right) \right] dt. \end{aligned}$$

In practice,  $\lambda_t$  is set to zero for sufficiently small  $t$  to avoid potential singularity issues. This leads to the following ERM (empirical risk minimization) estimator

$$\hat{\mathbf{f}} \in \underset{\mathbf{f} \in \mathcal{F}}{\text{argmin}} \frac{1}{n} \sum_{i=1}^n \ell_{\mathbf{f}}(\mathbf{X}^i), \quad (6)$$

where

$$\ell_{\mathbf{f}}(\mathbf{x}) = \int_{\underline{T}}^{\bar{T}} \lambda_t \mathbb{E} \left[ \left\| \mathbf{f}(\mathbf{X}_t, t) + \frac{\mathbf{X}_t - \mu_t \mathbf{X}_0}{\sigma_t^2} \right\|_2^2 \mid \mathbf{X}_0 = \mathbf{x} \right] dt \quad (7)$$

is the loss function and  $\underline{T} > 0$  is a sufficiently small number.

Let  $(\widehat{\mathbf{Y}}_t)_{t \in [0, \bar{T} - \underline{T}]}$  be the solution to the SDE

$$d\widehat{\mathbf{Y}}_t = \left[ \alpha_{\bar{T}-t} \widehat{\mathbf{Y}}_t + 2\alpha_{\bar{T}-t} \widehat{\mathbf{f}}(\widehat{\mathbf{Y}}_t, \bar{T} - t) \right] dt + \sqrt{2\alpha_{\bar{T}-t}} d\mathbf{B}_t, \quad \widehat{\mathbf{Y}}_0 \sim \mathcal{N}(\mathbf{0}_D, \mathbb{I}_D) \quad (8)$$

and  $\widehat{\mathbf{X}}_t = \widehat{\mathbf{Y}}_{\bar{T}-t}$ . Let  $\widehat{P}_t$  be the marginal distribution of  $\widehat{\mathbf{X}}_t$  and  $\widehat{p}_t$  be the corresponding Lebesgue density. Also, let  $\widehat{P} = \widehat{P}_{\bar{T}}$  and  $\widehat{p} = \widehat{p}_{\bar{T}}$ . The existence of  $\widehat{p}_t$  is guaranteed under mild assumptions; see Bogachev et al. (2011) for details. Although  $\widehat{p}_t$  is only defined implicitly through the SDE (8), it is a function of data, hence an estimator for the unknown density  $p_t$ . Since we expect that  $p_t \approx p_0$  for sufficiently small  $t$ ,  $\widehat{p}$  can serve as an estimator for  $p_0$ .

**Remark 1** *Note that the loss function (7) involves integrals (with respect to  $\mathbf{X}_t$  and  $t$ ) that are not directly tractable. In practice, a slightly different loss function with augmented variables is considered for computational tractability (Sohl-Dickstein et al., 2015; Song and Ermon, 2019). Specifically, with a slight abuse of notation, define the loss function*

$$\ell_{\mathbf{f}}(\mathbf{x}_0, \mathbf{x}_t, t) = \left\| \mathbf{f}(\mathbf{x}_t, t) + \frac{\mathbf{x}_t - \mu_t \mathbf{x}_0}{\sigma_t^2} \right\|_2^2.$$

By regarding  $T$  as a random variable independent of the stochastic process  $(\mathbf{X}_t)$  and supported on  $[\underline{T}, \bar{T}]$  with the density proportional to  $\lambda_t$ , we have

$$C_T \mathbb{E}[\ell_{\mathbf{f}}(\mathbf{X}_0, \mathbf{X}_T, T)] = \mathbb{E}[\ell_{\mathbf{f}}(\mathbf{X}_0)],$$

where  $C_T = \int_{\underline{T}}^{\bar{T}} \lambda_t dt$  is a normalizing constant. Therefore, although the loss function (7) itself is not directly tractable, one can approximate the solution to the minimization problem (6) using stochastic gradient methods.

**Remark 2** *The target estimator in our theoretical study in Section 5 is  $\widehat{p}$  as defined above, which is the density of  $\widehat{\mathbf{X}}_{\bar{T}} = \widehat{\mathbf{Y}}_{\bar{T}-\underline{T}}$ . In practice, samples from the estimated distribution are generated by numerically solving the SDE (8) using methods such as Euler-Maruyama discretization (Kloeden and Platen, 2011; Song et al., 2021), starting from an initial sample drawn from the standard normal distribution. Hence, more delicate statistical theory should incorporate these discretization errors. As an independent line of work, there are various articles studying discretization errors in diffusion models (Oko et al., 2023; Chen et al., 2023c; Nakano, 2024; Bortoli, 2022; Benton et al., 2024; Chen et al., 2023b; Li et al., 2024; Liang et al., 2025). Combining our statistical theory given in Section 5 with these works, the main results remain valid if the SDE is discretized with a sufficiently fine time partition. For additional details, we refer to Section 5.3 of Oko et al. (2023).*

### 3. Sparse Weight-Sharing Neural Networks

In this section, we define neural networks that are used as a function class  $\mathcal{F}$  to model the score function  $\mathbf{f}_0$  described in Section 2. Instead of vanilla feedforward neural networks, we consider sparse weight-sharing architectures, which are widely used in practical applications. By incorporating such sparsity and weight-sharing structures into the network architecture that models the score function, one can substantially reduce the model complexity (often expressed in terms of metric entropy; see Lemma 27), ultimately leading to a reduction in estimation error.

For a positive integer  $m$ , let  $\rho_m : \mathbb{R}^m \rightarrow \mathbb{R}^m$  be the coordinatewise ReLU activation function defined as  $\rho_m(\mathbf{z}) = (\max\{z_1, 0\}, \dots, \max\{z_m, 0\})^\top$  for  $\mathbf{z} = (z_1, \dots, z_m)^\top$ . For simplicity, we often denote  $\rho_m$  as  $\rho$ . For  $L \in \mathbb{N}_{\geq 2}$ ,  $\mathbf{d} = (d_1, \dots, d_{L+1}) \in \mathbb{N}^{L+1}$ ,  $s \in \mathbb{N}$ ,  $M > 0$ ,  $\mathbf{m} = (m_1, \dots, m_{L-1}) \in \mathbb{N}^{L-1}$  and

$$\mathcal{P}_{\mathbf{m}} = ((\mathcal{Q}_i, \mathcal{R}_i))_{i \in [L-1]},$$

where  $\mathcal{Q}_i = (Q_i^{(j)})_{j \in [m_i]}$  is a collection of  $d_i \times d_i$  permutation matrices and  $\mathcal{R}_i = (R_i^{(j)})_{j \in [m_i]}$  is a collection of  $d_{i+1} \times d_{i+1}$  permutation matrices, let  $\mathcal{F}_{\text{WSNN}} = \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  be the class of functions  $\mathbf{f} : \mathbb{R}^{d_1} \rightarrow \mathbb{R}^{d_{L+1}}$  of the form

$$\begin{aligned} \mathbf{f}(\mathbf{z}) &= W_L (\mathbf{f}_{L-1} \circ \dots \circ \mathbf{f}_1)(\mathbf{z}) + \mathbf{b}_L, \\ \mathbf{f}_i(\cdot) &= \rho \left( \sum_{j=1}^{m_i} R_i^{(j)} (W_i Q_i^{(j)} \cdot + \mathbf{b}_i) \right) \end{aligned} \quad (9)$$

with  $W_i \in \mathbb{R}^{d_{i+1} \times d_i}$  and  $\mathbf{b}_i \in \mathbb{R}^{d_{i+1}}$  satisfying

$$\max_{1 \leq i \leq L} \{\max(\|W_i\|_\infty, \|\mathbf{b}_i\|_\infty)\} \leq M, \quad \sum_{i=1}^L (\|W_i\|_0 + \|\mathbf{b}_i\|_0) \leq s.$$

Here,  $\|W_i\|_\infty$  and  $\|W_i\|_0$  denote the entrywise maximum norm and the number of nonzero elements of the matrix  $W_i$ , respectively.

The network (9) includes vanilla feedforward neural networks as special cases. For example, if  $\mathbf{m} = (1, \dots, 1)$  and all matrices in  $\mathcal{P}_{\mathbf{m}}$  are identity matrices, the class  $\mathcal{F}_{\text{WSNN}}$  reduces to the usual class of sparse networks considered in the literature. In this case, we often denote  $\mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  as  $\mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$ .

The network (9) is designed to incorporate sparsity and weight-sharing into the architecture. As a simple example, consider a weight matrix  $W \in \mathbb{R}^{3d \times 4d}$  with the following block structure, where each block has the same size of  $d \times d$ :

$$W = \begin{bmatrix} W_0 & 0_{d,d} & 0_{d,d} & W_0 \\ 0_{d,d} & 0_{d,d} & W_0 & 0_{d,d} \\ 0_{d,d} & W_0 & 0_{d,d} & W_0 \end{bmatrix}.$$

Here,  $0_{d,d}$  denotes the  $d \times d$  zero-matrix. Two important features of  $W$  are that it is sparse, in the sense that many elements of  $W$  are exactly zero, and that the sub-matrix  $W_0$  is shared across different rows and columns. The formula (9) is one way to effectively represent neural

networks with sparse weight-sharing matrices like  $W$ . For example, it is straightforward to construct  $3d \times 3d$  permutation matrices  $R^{(j)}$  and  $4d \times 4d$  permutation matrices  $Q^{(j)}$ , for  $j \leq 5$ , that satisfy

$$W = \sum_{j=1}^5 R^{(j)} \begin{bmatrix} W_0 & 0_{d,3d} \\ 0_{2d,d} & 0_{2d,3d} \end{bmatrix} Q^{(j)}.$$

The number of nonzero elements of  $W$  is  $5d^2$ , but we can express it with a smaller sparsity of  $d^2$  by weight-sharing architecture.

Sparse weight-sharing matrices are used in many practically important architectures, such as convolutional neural networks (LeCun et al., 1989; Krizhevsky et al., 2012) and recurrent neural networks (Rumelhart et al., 1986; Sutskever et al., 2014); see also Zhang et al. (2021) and Jagtap et al. (2022) for additional examples. Note that CNN architectures are frequently adopted in diffusion models (Sohl-Dickstein et al., 2015; Ho et al., 2020; Ronneberger et al., 2015).

As an illustrative example, consider a convolution operation with an input image  $\mathbf{x}$  of size  $d_1 = s_1^2$ , a filter of size  $s = s_0^2$ , and an output image  $\mathbf{y}$  of size  $d_2 = (s_1 - s_0 + 1)^2$ , as illustrated in Figure 1. Let  $\mathbf{w} = (w_1, \dots, w_s)^\top$  be the vectorized version of the filter, concatenating all columns of the filter sequentially, and let  $\widetilde{W} \in \mathbb{R}^{d_2 \times d_1}$  be the weight matrix corresponding to the convolution operation, such that  $\mathbf{y} = \widetilde{W}\mathbf{x}$ . One can observe that  $\widetilde{W}$  is a sparse weight-sharing matrix and can be represented in the form of (9). To see this, note that each row of  $\widetilde{W}$  can be obtained by permuting the vector  $(\mathbf{w}^\top, 0_{1,d_1-s}) \in \mathbb{R}^{d_1}$ . Thus, for  $j \in [d_2]$ , there exists a  $d_1 \times d_1$  permutation matrix  $Q^{(j)}$  such that  $y_j = (\mathbf{w}^\top, 0_{1,d_1-s})Q^{(j)}\mathbf{x}$ . Also, for  $j \in [d_2]$ , let  $R^{(j)}$  be the  $d_2 \times d_2$  permutation matrix that swaps the first and the  $j$ th row when it is left-multiplied by a matrix. Then, we can express the matrix  $\widetilde{W}$  in the form of (9) by

$$\widetilde{W} = \sum_{j=1}^{d_2} R^{(j)} W Q^{(j)}, \quad W = \begin{pmatrix} \mathbf{w}^\top & 0_{1,d_1-s} \\ 0_{d_2-1,s} & 0_{d_2-1,d_1-s} \end{pmatrix} \in \mathbb{R}^{d_2 \times d_1}.$$

One may additionally incorporate padding and stride operations (Paszke et al., 2019) into the convolution operation described in Figure 1. The corresponding weight matrix, with these additional operations, can also be expressed in the form of (9) by carefully selecting the permutation matrices.

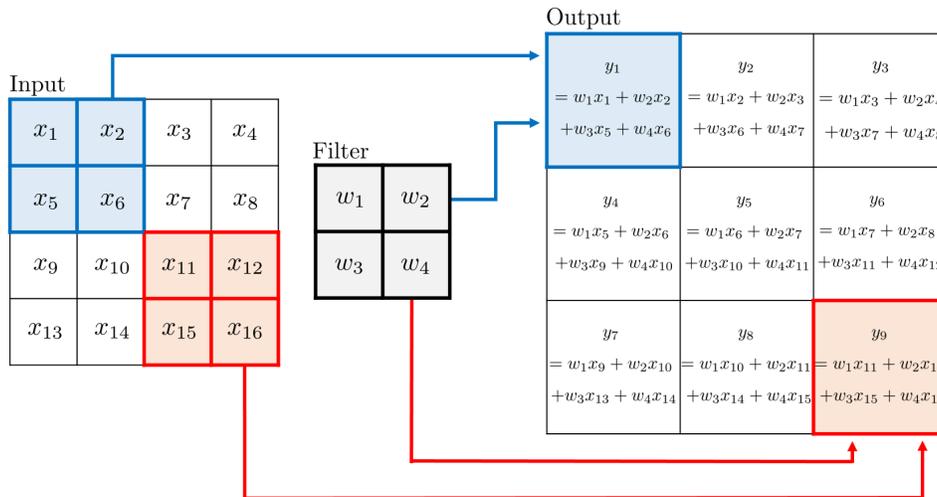
## 4. Factorizable Densities

### 4.1 Factorization Assumption

In this section, we introduce the low-dimensional assumption considered in our main results and provide some well-known examples. Formally, we consider the following factorization assumption.

(F) There exists a set  $\mathcal{I} \subseteq 2^{[D]}$  and functions  $g_I : \mathbb{R}^{|\mathcal{I}|} \rightarrow \mathbb{R}$  for each  $I \in \mathcal{I}$  such that

$$p_0(\mathbf{x}) = \prod_{I \in \mathcal{I}} g_I(\mathbf{x}_I), \quad \forall \mathbf{x} \in \mathbb{R}^D.$$



$$\widetilde{W} = \begin{pmatrix} w_1 & w_2 & 0 & 0 & w_3 & w_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & w_1 & w_2 & 0 & 0 & w_3 & w_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & w_1 & w_2 & 0 & 0 & w_3 & w_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w_1 & w_2 & 0 & 0 & w_3 & w_4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & w_1 & w_2 & 0 & 0 & w_3 & w_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_1 & w_2 & 0 & 0 & w_3 & w_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_1 & w_2 & 0 & 0 & w_3 & w_4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_1 & w_2 & 0 & 0 & w_3 & w_4 \end{pmatrix}$$

Figure 1: Example of a 2-dimensional convolution operation with an input  $\mathbf{x} \in \mathbb{R}^{16}$ , a filter vector  $\mathbf{w} \in \mathbb{R}^4$  and output  $\mathbf{y} \in \mathbb{R}^9$ . The operation can be represented as a matrix multiplication (Goodfellow et al., 2016), given by  $\mathbf{y} = \widetilde{W}\mathbf{x}$ .

For a density  $p_0$  satisfying **(F)**, let  $d = \max_{I \in \mathcal{I}} |I|$  denote the largest number of variables that any  $g_I$  depends on. We refer to  $d$  as the effective dimension corresponding to the factorizable density  $p_0$ . As a simple example, if  $p_0$  is the density of a random vector  $\mathbf{X} = (X_1, \dots, X_D)$  and each component of  $\mathbf{X}$  is mutually independent, then  $d = 1$ . In the following subsections, we present examples based on conditional independence structures, which are often represented using graphical models.

### 4.2 Example: Bayesian Networks

A Bayesian network is a random vector  $\mathbf{X} = (X_1, \dots, X_D)$  whose conditional independence structure can be represented by a directed acyclic graph (DAG) with the vertex set  $\{1, \dots, D\}$ . For a Bayesian network, each variable  $X_i$  is conditionally independent of all other variables given its parent variables  $\mathbf{X}_{\text{pa}(i)} = (X_j)_{j \in \text{pa}(i)}$ , where  $\text{pa}(i)$  denotes the set of parent indices of vertex  $i$ . Accordingly, the density  $p_0(\cdot)$  of a Bayesian network  $\mathbf{X}$  factorizes

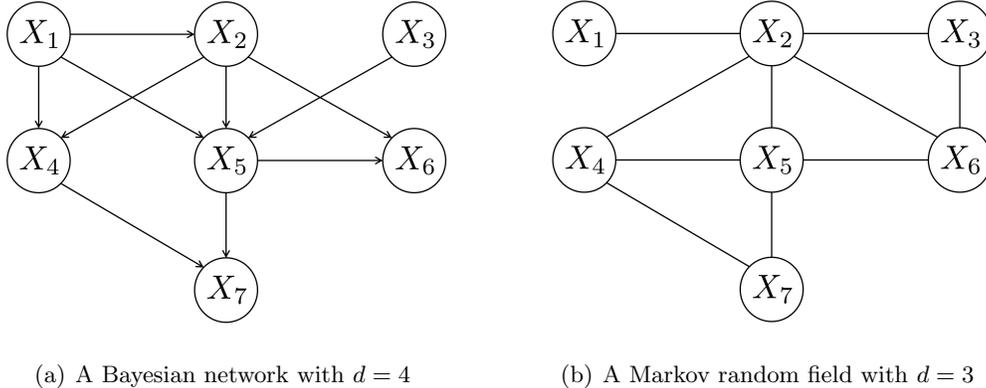


Figure 2: Examples of directed and undirected graphical model structures for a 7-dimensional random vector. In both cases, the effective dimension  $d$  is strictly less than  $D = 7$ .

as

$$p_0(\mathbf{x}) = \prod_{i=1}^D p_i(x_i | \mathbf{x}_{\text{pa}(i)}) = \prod_{i=1}^D g_i(x_i, \mathbf{x}_{\text{pa}(i)}),$$

where  $p_i(\cdot | \mathbf{x}_{\text{pa}(i)})$  is the conditional density of  $X_i$  given  $\mathbf{X}_{\text{pa}(i)} = \mathbf{x}_{\text{pa}(i)}$  and  $g_i(x_i, \mathbf{x}_{\text{pa}(i)}) = p_i(x_i | \mathbf{x}_{\text{pa}(i)})$ . Hence,  $p_0$  satisfies the assumption **(F)** with  $\mathcal{I} = \{\{i\} \cup \text{pa}(i) : i \in [D]\}$  and  $d = 1 + \max_{i \in [D]} |\text{pa}(i)|$ ; see Figure 2(a) for an illustrative example.

### 4.3 Example: Markov Random Fields

A Markov random field over an undirected graph  $G$  with vertex set  $\{1, \dots, D\}$  is a random vector  $\mathbf{X} = (X_1, \dots, X_D)$  with the property that each variable  $X_i$  is conditionally independent of all other variables given its neighbors, often referred to as the local Markov property (Lauritzen, 1996). If the density  $p_0(\cdot)$  of  $\mathbf{X}$  is strictly positive, the local Markov property holds if and only if

$$p_0(\mathbf{x}) = \prod_{C \in \mathcal{C}} g_C(\mathbf{x}_C) \quad (10)$$

for some functions  $g_C$ , where  $\mathcal{C}$  denotes the set of all (maximal) cliques in the graph, as stated by the celebrated Hammersley-Clifford theorem (Hammersley and Clifford, 1971; Lauritzen, 1996). Here, a clique is a fully connected subset of the vertex set in a graph, and the factors  $g_C$  are referred to as potential functions in Markov random fields. Therefore, the assumption **(F)** holds with  $\mathcal{I} = \mathcal{C}$  and  $d = \max_{C \in \mathcal{C}} |C|$ , where  $d$  represents the maximum number of vertices in the (maximal) cliques; see Figure 2(b) for an illustrative example.

Note that images consist of pixels with strong spatial correlations. It is, therefore, natural to assume that each pixel is conditionally independent of all other pixels given the pixels in its neighborhood. This makes the local Markov property particularly suitable for

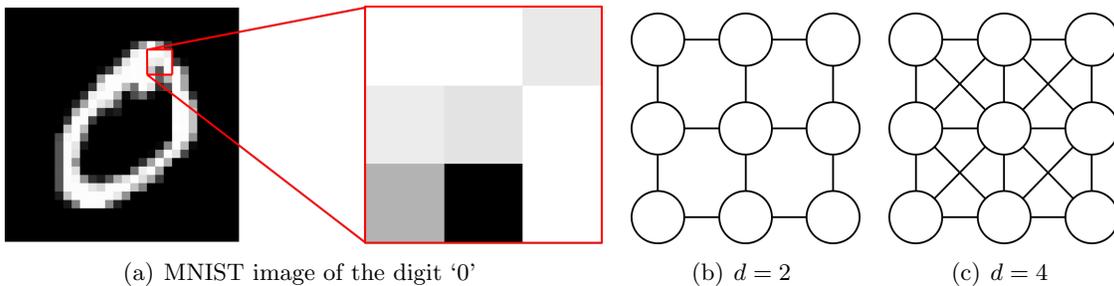


Figure 3: An image of the digit ‘0’ from the MNIST data set (LeCun et al., 1998), along with two possible undirected graph structures for MNIST. For each pixel, a larger neighborhood may be considered depending on the degree of spatial correlations.

image data. For example, one might consider a graphical model structure, such as in Figure 3(b), which has a very small  $d$  (e.g.,  $d = 2$  in this example).

## 5. Main Results

In this section, we present the main results of the paper. Section 5.1 introduces the assumptions on  $p_0$  required for the main results. Section 5.2 presents our main theorem (Theorem 3), which establishes the convergence rate of the diffusion estimator  $\hat{p}$  introduced in Section 2. Finally, Section 5.3 describes the key technical components used to prove Theorem 3, namely the approximation of the score function  $\mathbf{f}_0$  using sparse weight-sharing neural networks.

### 5.1 Assumptions

For given data  $\mathbf{X}^1, \dots, \mathbf{X}^n$ , let  $\hat{p}$  and  $(\hat{p}_t)$  be defined as in Section 2. Note that the estimators  $\hat{p}$  and  $(\hat{p}_t)$  depend only on the non-random quantities  $(\alpha_t)$ ,  $(\lambda_t)$ ,  $\bar{T}$ ,  $\underline{T}$  (which may depend on the sample size  $n$ ), and the architecture  $\mathcal{F} = \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$ . Recall that  $\alpha_t$  is the negative drift coefficient of the forward diffusion (2),  $\lambda_t$  is the weight for the loss function (7), and  $[\underline{T}, \bar{T}]$  is the interval defining both the loss function and the estimator  $\hat{p}$ . Throughout the paper, we assume the following without explicit restatement:

1.  $\mathbf{X}^1, \dots, \mathbf{X}^n$  are i.i.d. from  $p_0$ , supported on  $[-1, 1]^D$ .
2.  $\sup_{\gamma \in \mathbb{N}} |\partial^\gamma \alpha_t / \partial t^\gamma| \leq 1$  for all  $t \geq 0$  and  $\underline{\tau} \leq \alpha_t \leq \bar{\tau}$  for constants  $\underline{\tau}, \bar{\tau} > 0$ .
3.  $\lambda_t = 1$  for all  $t \geq \underline{T}$ .

Note that the standard OU process corresponds to  $\alpha_t = 1$ , and widely used diffusion models in practice (DDPM; Ho et al., 2020) often set  $t \mapsto \alpha_t$  as a linear function; both choices satisfy the above requirements. For simplicity of the proofs, we set the weight function  $\lambda_t$  to be constant. We also note that, with additional technical details, our main results can be extended to more general choices of forward diffusion processes and weight

functions. For various designs of such choices in practice, we refer to Karras et al. (2022). In addition to these basic assumptions, we will require the following additional assumptions:

- (S) The factorization assumption (F) is satisfied and there exist constants  $\beta, K > 0$  such that  $p_0 \in \mathcal{H}^{\beta, K}([-1, 1]^D)$  and  $g_I \in \mathcal{H}^{\beta, K}([-1, 1]^{|I|})$  for every  $I \in \mathcal{I}$ .
- (L) There exists a constant  $\tau_1 > 0$  such that  $p_0(\mathbf{x}) \geq \tau_1$  for every  $\mathbf{x} \in [-1, 1]^D$ .
- (B) In addition to (S), there exists a constant  $\tau_2 \in (0, 1)$  such that

$$\sup_{\gamma \in \mathbb{N}^D} \sup_{\mathbf{x}: 1 - \tau_2 \leq \|\mathbf{x}\|_\infty \leq 1} |\mathbb{D}^\gamma p_0(\mathbf{x})| \leq K.$$

As in Oko et al. (2023), assumptions (B) and (L) are imposed purely for technical convenience. Although assuming that the density vanishes near the boundary of its support is more natural and plausible, assumption (L) greatly simplifies many proofs related to score-function estimation, since the score function  $\nabla \log p_t(\mathbf{x})$  is defined as the ratio  $\nabla p_t(\mathbf{x})/p_t(\mathbf{x})$ . For this reason, following Oko et al. (2023), we adopted this assumption for tractability.

It should be noted that assumption (L) conflicts with the regularity or smoothness condition: once the density is bounded from below by a positive constant on its support, it automatically becomes non-smooth near the boundary when viewed as a function on  $\mathbb{R}^D$ . This irregularity necessitates a careful approximation analysis near the boundary. To facilitate this analysis, we introduced the technical assumption (B), again following Oko et al. (2023). We also note that our main result, Theorem 3, remains valid if the constant  $\tau_2$  in assumption (B) is replaced by  $(\log n)^{-\tau_{\text{bd}}}$ , where  $\tau_{\text{bd}}$  is an arbitrarily large constant.

In a recent preprint, Fan et al. (2025) obtained similar results without assumption (B), and their approach could, in principle, be adapted to our framework to remove (B) as well. We also note that several recent works (Zhang et al., 2024; Wibisono et al., 2024; Fu and Lee, 2025) have established results comparable to or weaker than those of Oko et al. (2023) without relying on assumptions (B) and (L). However, their techniques do not appear to extend easily to the setting of factorizable densities considered in our paper.

The factorization assumption (F), combined with the smooth components assumption (S), forms the key structural assumption for our main results. Note that our results can be easily extended to the case where each factor function possesses a different level of smoothness. The factorization assumption with smooth nonparametric components has been investigated in the statistical literature under the framework of nonparametric graphical models, specifically in the Markov random fields. Liu et al. (2011), Liu et al. (2012), Györfi et al. (2023) focused on undirected acyclic graphs (forests), where  $d$  is at most 2, and employed kernel methods. With this simple graph structure, Liu et al. (2011) developed a consistent graph selection method, while Liu et al. (2012) constructed a minimax optimal density estimator for the special case of  $\beta = 2$ . Further advancements for the case  $\beta = 1$  were studied in Györfi et al. (2023).

Nonparametric statistical theory for general undirected graph structures has been studied in some recent articles. In the case of  $\beta = 1$ , Vandermeulen et al. (2024a) and Vandermeulen et al. (2024b) proposed estimators whose convergence rates do not depend on the data dimension  $D$ . More specifically, Vandermeulen et al. (2024a) introduced a novel quantity called the graph resilience  $r$  and derived a convergence rate of  $n^{-1/(r+2)}$  (up to

a logarithmic factor) with respect to the total variation distance. They showed that this quantity satisfies  $d \leq r \leq D$ , meaning their rate is optimal only in special cases where  $d = r$ . Notably,  $r$  can be much larger than  $d$ , for example, when the graph is a tree. Van-dermeulen et al. (2024b) studied a more tractable DNN-based estimator with a convergence rate of  $n^{-1/(d+4)}$ , which is sub-optimal. More recently, Gottwald et al. (2025) introduced a quantitative condition that characterizes the locality structure of the graph. They further showed that diffusion models yield consistent estimators when  $D \gtrsim \log n$ , with convergence rates that depend on this additional locality structure.

Bos and Schmidt-Hieber (2024) considered a slightly more general structure than the factorization assumption **(F)**, using a different type of estimator. Specifically, they assumed that  $p_0$  has a composite structure with smooth component functions. It is well known that deep neural networks can adapt to composite structures in nonparametric function estimation; see Schmidt-Hieber (2020), Bauer and Kohler (2019), and Kohler and Langer (2021). Bos and Schmidt-Hieber (2024) transformed the density estimation problem into a nonparametric regression problem and then constructed a density estimator. With this approach, they achieved a convergence rate of  $n^{-\beta/(d+2\beta)} \vee n^{-\beta/D}$  (up to a logarithmic factor). While this rate improves upon existing results, it is optimal only when  $D \leq 2\beta + d$ . Note that our main results can also be extended to the composite structure considered in Bos and Schmidt-Hieber (2024) without significant difficulty.

## 5.2 Convergence Rate

The total variation distance between two Borel probability measures  $P$  and  $Q$  on  $\mathbb{R}^D$  is defined as

$$d_{\text{TV}}(P, Q) = \sup_A |P(A) - Q(A)|,$$

where the supremum is taken over every Borel subset  $A$  of  $\mathbb{R}^D$ . We often denote  $d_{\text{TV}}(P, Q)$  as  $d_{\text{TV}}(p, q)$ , where  $p$  and  $q$  are Lebesgue densities of  $P$  and  $Q$ , respectively. The following theorem provides the convergence rate of  $\hat{p}$  with respect to the total variation, which is our main result. Recall the definitions of the estimators  $\hat{\mathbf{f}}$  and  $\hat{p}$  from Section 2, and note that the score function is denoted by  $\mathbf{f}_0(\mathbf{x}, t) = \nabla \log p_t(\mathbf{x})$ .

**Theorem 3** *Suppose that  $p_0$  satisfies **(S)**, **(L)**, and **(B)**. Let  $\tau_{\min}$  and  $\tau_{\max}$  be constants with*

$$\tau_{\min} \geq \frac{d}{2\beta + d} \left( \frac{4\beta}{d(\beta \wedge 1)} \vee \frac{1}{3D} \right) \quad \text{and} \quad \tau_{\max} \geq \frac{\beta}{\underline{T}(2\beta + d)} \vee \frac{2dD}{(2\beta + d)\bar{T}}.$$

*Let  $\underline{T} = n^{-\tau_{\min}}$  and  $\bar{T} = \tau_{\max} \log n$ . Then, for every  $n \geq C_2$ , there exist a collection of permutation matrices  $\mathcal{P}_{\mathbf{m}} = ((\mathcal{Q}_i, \mathcal{R}_i))_{i \in [L-1]}$  and a class of weight-sharing neural networks  $\mathcal{F}_{\text{WSNN}} = \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  with*

$$\begin{aligned} L &\leq C_1 (\log n)^6 \log \log n, & \|\mathbf{d}\|_{\infty} &\leq C_1 n^{\frac{d(D+1)}{2\beta+d}}, \\ s &\leq C_1 n^{\frac{d}{2\beta+d}} (\log n)^5 \log \log n, & M &\leq \exp(C_1 \{\log n\}^6), \\ \|\mathbf{m}\|_{\infty} &\leq C_1 n^{\frac{dD}{2\beta+d}} \end{aligned}$$

satisfying

$$\mathbb{E} \left[ \left( \int_{\underline{T}}^{\bar{T}} \int_{\mathbb{R}^D} \|\widehat{\mathbf{f}}(\mathbf{x}, t) - \mathbf{f}_0(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} dt \right)^{1/2} \right] \leq \epsilon_n,$$

where  $\widehat{\mathbf{f}}$  is the ERM estimator over the class  $\mathcal{F} = \mathcal{F}_{\text{WSNN}} \cap \mathcal{F}_\infty$  with

$$\mathcal{F}_\infty = \left\{ \mathbf{f} : \|\mathbf{f}(\mathbf{x}, t)\|_\infty \leq \frac{C_1 \sqrt{\log n}}{\sigma_t} \quad \forall \mathbf{x} \in \mathbb{R}^D, t > 0 \right\}$$

and

$$\epsilon_n = C_1 n^{-\frac{\beta}{2\beta+d}} \left\{ (\log n)^{2D+2\beta+1} + (\log n)^{10} \right\}.$$

Moreover,

$$\mathbb{E} [d_{\text{TV}}(p_0, \widehat{p})] \leq \epsilon_n,$$

where  $\widehat{p} = \widehat{p}_{\underline{T}}$  is the corresponding estimator defined through the SDE (8). Here,  $C_1, C_2$  are constants depending only on  $(\beta, d, D, K, \tau_{\min}, \tau_{\max}, \tau_1, \tau_2, \bar{\tau}, \underline{T})$ .

The proof of Theorem 3 is provided in the Appendix. Note that  $\bar{\tau}$  and  $\underline{T}$  can be treated as known constants. For example, if  $\alpha_t = 1$  for all  $t$ , both constants can be set to 1. The constants  $\tau_{\min}$  and  $\tau_{\max}$  can also be chosen to depend solely on the single quantity  $\beta/d$ , ignoring their dependence on the known quantities  $(D, \bar{\tau}, \underline{T})$ .

It can be observed that the class of permutation matrices  $\mathcal{P}_{\mathbf{m}}$  can likewise be chosen to depend only on  $\beta/d$ ; see Section 5.3 for details. Similarly, if  $\tau_1, \tau_2$ , and  $K$  are treated as known constants, the hyperparameters  $(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  defining the neural network  $\mathcal{F}_{\text{WSNN}}$  can also be selected to depend solely on  $\beta/d$ . Therefore, the estimators  $\widehat{\mathbf{f}}$  and  $\widehat{p}$  ultimately depend only on  $\beta/d$ .

In this sense,  $\widehat{\mathbf{f}}$  and  $\widehat{p}$  are adaptive to the factorization structure because their construction does not rely on the structural information. We do not aim in this paper to construct a fully adaptive estimator, in the sense of estimators that do not depend on  $\beta/d$ . Although the architectures in Theorem 3, including the class  $\mathcal{P}_{\mathbf{m}}$  of permutation matrices and the hyperparameters  $(L, \mathbf{d}, s, M)$ , can be chosen to depend solely on  $\beta/d$ , in practice, much more complex architectures are often used, and hyperparameters are carefully tuned based on extensive experimental work.

Note that the convergence rate in Theorem 3 is minimax-optimal up to a logarithm factor over the class of factorizable densities. Specifically, for  $\beta, K > 0$  and  $D, d \in \mathbb{N}$  with  $d \leq D$ , let

$$\mathcal{G}(\beta, D, d, K) = \left\{ g_0 \in \mathcal{H}^{\beta, K}([-1, 1]^D) : g_0(\mathbf{x}) = \prod_{I \in \mathcal{I}} g_I(\mathbf{x}_I), \right. \\ \left. g_I \in \mathcal{H}^{\beta, K}([-1, 1]^{|I|}), \max_{I \in \mathcal{I}} |I| = d, \mathcal{I} \subseteq 2^{[D]} \right\} \quad (11)$$

be the class of factorizable densities with smooth component functions. Then, we have

$$\inf_{\widehat{p}} \sup_{p_0 \in \mathcal{G}(\beta, D, d, K)} \mathbb{E}[d_{\text{TV}}(p_0, \widehat{p})] \gtrsim n^{-\beta/(2\beta+d)},$$

where the infimum is taken over all estimators. The proof of this lower bound is straightforward, given the well-known result that the minimax rate for estimating a  $d$ -dimensional density in  $\mathcal{H}^{\beta, K}([-1, 1]^d)$  is  $n^{-\beta/(2\beta+d)}$  (Giné and Nickl, 2016).

Here, we present an overview of the key ideas behind the proof. Recall that  $\widehat{p} = \widehat{p}_{\underline{T}}$ . By the triangle inequality, we have

$$\mathbb{E}[d_{\text{TV}}(p_0, \widehat{p})] \leq d_{\text{TV}}(p_0, p_{\underline{T}}) + \mathbb{E}[d_{\text{TV}}(p_{\underline{T}}, \widehat{p}_{\underline{T}})]. \quad (12)$$

The first term in the right-hand side of (12) scales as a polynomial order in  $\underline{T} = n^{-\tau_{\min}}$ , thus we can control the error by choosing a large constant  $\tau_{\min}$ ; see Lemma 26 for details. The second term is the total variation distance between the distributions of  $\mathbf{X}_{\underline{T}} = \mathbf{Y}_{\overline{T}-\underline{T}}$  and  $\widehat{\mathbf{X}}_{\underline{T}} = \widehat{\mathbf{Y}}_{\overline{T}-\underline{T}}$ . Note that the two processes  $(\mathbf{Y}_t)_{t \in [0, \overline{T}]}$  and  $(\widehat{\mathbf{Y}}_t)_{t \in [0, \overline{T}]}$  differ only in their initial distributions and drift functions. Hence, based on well-known results, we can bound the total variation distance by controlling each difference separately as follows:

$$\begin{aligned} & \mathbb{E}[d_{\text{TV}}(p_{\underline{T}}, \widehat{p}_{\underline{T}})] \\ & \leq d_{\text{TV}}(P_{\overline{T}}, \mathcal{N}(\mathbf{0}_D, \mathbb{I}_D)) + \mathbb{E} \left[ \left( \int_{\underline{T}}^{\overline{T}} \int_{\mathbb{R}^D} 4\alpha_t \left\| \widehat{\mathbf{f}}(\mathbf{x}, t) - \mathbf{f}_0(\mathbf{x}, t) \right\|_2^2 p_t(\mathbf{x}) d\mathbf{x} dt \right)^{1/2} \right]; \end{aligned} \quad (13)$$

see Remark 2.3 of Bogachev et al. (2016). Both terms on the right-hand side of (13) correspond to the differences between the initial distributions and the drift functions, respectively. The first term can be easily controlled because  $P_{\overline{T}}$  converges exponentially fast to  $\mathcal{N}(\mathbf{0}_D, \mathbb{I}_D)$  as  $\overline{T} = \tau_{\max} \log n$  increases. Thus, we can control the error by choosing a large constant  $\tau_{\max}$ .

The second term on the right-hand side of (13) represents the risk of the empirical risk minimizer  $\widehat{\mathbf{f}}$ ; see Proposition 29 for the detailed statement regarding this term. There is a substantial body of literature introducing techniques to bound the risk of empirical risk minimizers (e.g., van der Vaart and Wellner, 1996; van de Geer, 2000; Wainwright, 2019). Technically, the risk can be decomposed into two terms: the approximation error and the estimation error, often referred to as the bias-variance decomposition. To bound the estimation error, the key is to control the metric entropy of the weight-sharing networks  $\mathcal{F}_{\text{WSNN}}$ ; see Lemma 27 for details. The key technical contribution of our work lies in developing a sharp approximation error bound for score functions under the factorization assumption **(F)**, which is introduced in the following subsection.

**Remark 4** *In **(S)**, we assume that all factors  $g_I$  have the same smoothness level. This assumption can be relaxed, allowing each  $g_I$  to have a different level of smoothness. Specifically, suppose that for each  $I \in \mathcal{I}$ , we have  $g_I \in \mathcal{H}^{\beta_I, K}([-1, 1]^{|I|})$  for some  $\beta_I > 0$ .*

*One can directly extend the proof of Theorem 3 to show that*

$$\mathbb{E}[d_{\text{TV}}(p_0, \widehat{p})] \lesssim_{\log} n^{-\frac{\beta_*}{2\beta_*+d_*}}$$

with a carefully chosen network architecture, where

$$I_* = \operatorname{argmin}_{I \in \mathcal{I}} \frac{\beta_I}{|I|}, \quad \beta_* = \beta_{I_*}, \quad d_* = |I_*|.$$

The set-up of different smoothness levels includes the case of Liu et al. (2007), who considered a density of the form  $p_0(\mathbf{x}) = g_I(\mathbf{x}_I)g_0(\mathbf{x})$ , where  $g_0$  is very smooth and  $I \subseteq [D]$ . Under the assumption that  $g_I$  has continuous second-order derivatives, they proposed a density estimator that achieves a convergence rate of  $O(n^{-2/(4+|I|)+\epsilon})$  for any  $\epsilon > 0$ .

### 5.3 Approximation Theory

Theorem 5 below presents the approximation results for the map  $(\mathbf{x}, t) \mapsto \mathbf{f}_0(\mathbf{x}, t) = \nabla \log p_t(\mathbf{x})$  using weight-sharing neural networks, which serves as the key technical component of our main results.

**Theorem 5** *Suppose the density function  $p_0$  satisfies the assumptions **(S)**, **(L)**, and **(B)**. Let  $\tau_{\min}$  and  $\tau_{\max}$  be constants with*

$$\tau_{\min} \geq \frac{4\beta}{d(\beta \wedge 1)} \vee \frac{1}{3D} \quad \text{and} \quad \tau_{\max} \geq \frac{2D}{\bar{\tau}}.$$

Then, for every  $m \geq C_4$ , there exist a collection of permutation matrices

$$\mathcal{P}_{\mathbf{m}} = ((\mathcal{Q}_i, \mathcal{R}_i))_{i \in [L-1]}$$

and a class of weight-sharing neural networks  $\mathcal{F}_{\text{WSNN}} = \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  with

$$\begin{aligned} L &\leq C_3(\log m)^6 \log \log m, & \|\mathbf{d}\|_{\infty} &\leq C_3 m^{D+1}, \\ s &\leq C_3 m(\log m)^5 \log \log m, & M &\leq \exp(C_3 \{\log m\}^6), \\ \|\mathbf{m}\|_{\infty} &\leq C_3 m^D \end{aligned}$$

such that

$$\inf_{\mathbf{f} \in \mathcal{F}_{\text{WSNN}} \cap \mathcal{F}_{\infty}} \int_{\underline{T}}^{\bar{T}} \int_{\mathbb{R}^D} \|\mathbf{f}_0(\mathbf{x}, t) - \mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} dt \leq C_3 m^{-\frac{2\beta}{d}} (\log m)^{4D+4\beta+1},$$

where  $\underline{T} = m^{-\tau_{\min}}$ ,  $\bar{T} = \tau_{\max} \log m$  and

$$\mathcal{F}_{\infty} = \left\{ \mathbf{f} : \|\mathbf{f}(\mathbf{x}, t)\|_{\infty} \leq \frac{C_3 \sqrt{\log m}}{\sigma_t} \quad \forall \mathbf{x} \in \mathbb{R}^D, t > 0 \right\}.$$

Here,  $C_3$  and  $C_4$  are constants depending only on  $(\beta, d, D, K, \tau_{\min}, \tau_{\max}, \tau_1, \tau_2, \bar{\tau}, \underline{T})$ .

The proof of Theorem 5 is provided in Appendix. From this proof, it can be deduced that the class of permutation matrices  $\mathcal{P}_{\mathbf{m}}$  can be chosen to depend only on  $m$  and  $\beta/d$ . In the proof of Theorem 3, we select  $m$  based solely on  $\beta/d$ , implying that the choice of  $\mathcal{P}_{\mathbf{m}}$  ultimately depends only on  $\beta/d$ .

Here, we present an overview of the key ideas behind the proof. Note that  $\nabla \log p_t(\mathbf{x}) = \nabla p_t(\mathbf{x})/p_t(\mathbf{x})$ , and the division operation can be approximated by DNNs very efficiently, provided that the denominator is not too small; see Lemma F.7 of Oko et al. (2023). Since the ideas behind approximating the maps  $(\mathbf{x}, t) \mapsto p_t(\mathbf{x})$  and  $(\mathbf{x}, t) \mapsto \nabla p_t(\mathbf{x})$  are similar, we only present the key idea for approximating  $(\mathbf{x}, t) \mapsto p_t(\mathbf{x})$ . For convenience, we use the informal notation  $a \lesssim_{\log} b$  to indicate that  $a$  is less than  $b$  up to a poly-logarithmic factor, such as  $\log n$ ,  $(\log m)^2$ , or  $\log(1/\sigma_t)$ . Similarly, we use the notation  $\asymp_{\log}$  to correspond to  $\lesssim$ .

For a given (sufficiently large) positive integer  $m$ , which roughly corresponds to the order of the number of nonzero network parameters, we will construct DNN approximators for the map  $(\mathbf{x}, t) \mapsto p_t(\mathbf{x})$  in four regions and combine them. These four regions for  $(\mathbf{x}, t)$  can be roughly defined as follows:

$$(R1) \text{ (Outside of near-support) } \|\mathbf{x}\|_{\infty} - \mu_t \gtrsim \sigma_t \sqrt{\log m}$$

$$(R2) \text{ (large } t) \|\mathbf{x}\|_{\infty} - \mu_t \lesssim \sigma_t \sqrt{\log m} \text{ and } t \gtrsim m^{-(2-\delta)/D} \text{ for some } \delta > 0$$

$$(R3) \text{ (Boundary of near-support) } t \lesssim m^{-(2-\delta)/D} \text{ and } -\{\log(1/\sigma_t)\}^{-3/2} \lesssim \|\mathbf{x}\|_{\infty} - \mu_t \lesssim \sigma_t \sqrt{\log m}$$

$$(R4) \text{ (Interior of near-support) } t \lesssim m^{-(2-\delta)/D} \text{ and } \|\mathbf{x}\|_{\infty} - \mu_t \lesssim -\{\log(1/\sigma_t)\}^{-3/2}$$

Recall that  $\mu_t = \exp(-\int_0^t \alpha_s ds)$  and  $\sigma_t = \sqrt{1 - \mu_t^2}$ , so the maps  $t \mapsto \mu_t$  and  $t \mapsto \sigma_t$  can be approximated by DNNs very efficiently. Likewise, the map  $\mathbf{x} \mapsto \|\mathbf{x}\|_{\infty}$  can also be efficiently approximated. Therefore, once we can approximate the map  $(\mathbf{x}, t) \mapsto p_t(\mathbf{x})$  in each of the four regions, it is not difficult to combine them into a single function over the entire region.

In region (R1),  $p_t$  is nearly zero due to the sub-Gaussianity of  $p_t$ , making it easy to approximate. In region (R2),  $t$  is sufficiently large, and thus the map  $\mathbf{x} \mapsto p_t(\mathbf{x})$  is much smoother than  $\mathbf{x} \mapsto p_0(\mathbf{x})$ . This smoothness property enables the construction of a DNN with a moderate number of nonzero parameters, as in Lemma B.7 of Oko et al. (2023); see Proposition 25 for details. Similarly, in region (R3), the map  $\mathbf{x} \mapsto p_t(\mathbf{x})$  is very smooth due to the assumption **(B)**, allowing us to construct a DNN with the desired approximation properties, similar to Lemmas B.2–B.5 of Oko et al. (2023); see Proposition 24 for details.

The main challenge in the proof of Theorem 5 lies in the approximation in region (R4). Note that  $p_t(\mathbf{x}) \gtrsim 1$  in region (R4), and that

$$\begin{aligned} p_t(\mathbf{x}) &= \int_{\|\mathbf{z}\|_{\infty} \leq 1} p_0(\mathbf{z}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{z}) d\mathbf{z} \\ &= \int_{\left\| \frac{\mathbf{x} + \sigma_t \mathbf{y}}{\mu_t} \right\|_{\infty} \leq 1} \mu_t^{-D} p_0\left(\frac{\mathbf{x} + \sigma_t \mathbf{y}}{\mu_t}\right) \phi_1(\mathbf{y}) d\mathbf{y}, \end{aligned} \tag{14}$$

where  $\phi_{\sigma}$  denotes the density of  $\mathcal{N}(\mathbf{0}_D, \sigma^2 \mathbb{I}_D)$  for  $\sigma > 0$ . To approximate the right-hand side of (14), we first approximate it by a finite sum via a quadrature method, and then approximate the sum using a weight-sharing neural network.

To grasp the idea of approximation, it suffices to consider the approximation of a general function

$$\mathbf{x} \mapsto \int_{[-1,1]^D} g(\mathbf{x}, \mathbf{y}) d\mathbf{y}, \tag{15}$$

defined through a  $D$ -dimensional integral. Here,  $g$  is a function such that for each  $\mathbf{x}$ , the map  $\mathbf{y} \mapsto g(\mathbf{x}, \mathbf{y})$  belongs to  $\mathcal{H}^{\beta, K}([-1, 1]^D)$ , where  $K > 0$  is a constant independent of  $\mathbf{x}$ . We provide an idea for constructing a weight-sharing neural network to approximate the map (15) with an error of  $\epsilon \asymp_{\log} m^{-\beta/d}$ . It is well-known from numerical analysis (Novak, 1988) that, to achieve an approximation error of  $\epsilon$  for every function in  $\mathcal{H}^{\beta, K}([-1, 1]^D)$  using the Gauss–Legendre quadrature method, at least  $O(\epsilon^{-D/\beta})$  quadrature points are necessary. Hence, (15) can be approximated by a finite sum with  $O(\epsilon^{-D/\beta})$  summands. However, to approximate this  $O(\epsilon^{-D/\beta})$ -term summation using DNNs, we would need at least  $O(\epsilon^{-D/\beta})$  network parameters (up to a poly-logarithmic factor), which results in a very large estimation error. To overcome this difficulty, instead of applying a single  $D$ -dimensional quadrature method, we apply a 1-dimensional  $m$ -point quadrature method  $D$  times to approximate the  $D$ -dimensional integral (15). Specifically, let  $(w_j)_{j \in [m]}$  and  $(y_j)_{j \in [m]}$  be the  $m$ -point quadrature weights and nodes for 1-dimensional integrals over the interval  $[-1, 1]$ , that is, for any  $h \in \mathcal{H}^{\beta, K}([-1, 1])$ ,

$$\left| \int_{-1}^1 h(y) dy - \sum_{j=1}^m w_j h(y_j) \right| \lesssim m^{-\beta};$$

see Lemma 20 for details. Then, we can easily see that

$$\left| \int_{[-1, 1]^D} g(\mathbf{x}, \mathbf{y}) d\mathbf{y} - \sum_{\mathbf{j} \in [m]^D} w_{\mathbf{j}} g(\mathbf{x}, \mathbf{y}_{\mathbf{j}}) \right| \lesssim m^{-\beta}$$

where  $w_{\mathbf{j}} = \prod_{k=1}^D w_{j_k}$  and  $\mathbf{y}_{\mathbf{j}} = (y_{j_1}, \dots, y_{j_D})$ . Here, we slightly abuse the notation for weights.

We next approximate the map

$$\mathbf{x} \mapsto \sum_{\mathbf{j} \in [m]^D} w_{\mathbf{j}} g(\mathbf{x}, \mathbf{y}_{\mathbf{j}}) \tag{16}$$

using weight-sharing neural networks. Although the summation in (16) consists of  $m^D$  terms and resembles a  $m^D$ -point,  $D$ -dimensional quadrature, it can be approximated by weight-sharing DNNs much more efficiently than a standard  $m^D$ -point,  $D$ -dimensional quadrature approximation. The key ingredients are the approximations of the following two maps:

$$\begin{aligned} (w_1, \dots, w_m) &\mapsto (w_{\mathbf{j}})_{\mathbf{j} \in [m]^D} : \mathbb{R}^m \rightarrow \mathbb{R}^{m^D} \\ (\mathbf{x}, y_1, \dots, y_m) &\mapsto (g(\mathbf{x}, \mathbf{y}_{\mathbf{j}}))_{\mathbf{j} \in [m]^D} : \mathbb{R}^{D+m} \rightarrow \mathbb{R}^{m^D}. \end{aligned} \tag{17}$$

Although the  $w_{\mathbf{j}}$ 's are distinct, each  $w_{\mathbf{j}}$  is represented as a product of  $D$  terms from the  $m$  distinct values  $w_1, \dots, w_m$ . Therefore, to approximate the first map of (17), we only need to approximate the multiplication operation  $(x, y) \mapsto xy$  and apply it multiple times. Note that multiplication can be approximated by DNNs very efficiently (Schmidt-Hieber, 2020). With an additional trick, the repeated application of multiplication can be represented as a DNN of the form (9), with a suitable choice of permutation matrices. Roughly speaking, to achieve an approximation error of  $\epsilon \asymp_{\log} m^{-\beta/d}$  for this map, we only need  $O(\log m)$

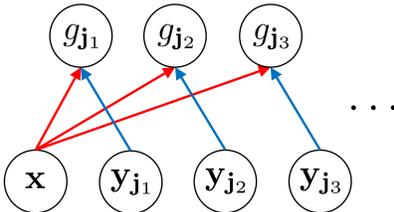


Figure 4: An illustration of why weight-sharing helps reduce model complexity: At some middle layers of the network, we need to approximate a map with inputs  $\mathbf{x}$  and  $\mathbf{y}_{\mathbf{j}}$ ,  $\mathbf{j} \in [m]^D$ , and outputs  $g_{\mathbf{j}} = g(\mathbf{x}, \mathbf{y}_{\mathbf{j}})$ ,  $\mathbf{j} \in [m]^D$ . Since a single function  $g$  is approximated for  $m^D$  instances, leaving all network parameters as free parameters is inefficient. Weight-sharing can significantly reduce the number of distinct parameters. In this illustration, all edges with the same color share the same weight parameters.

distinct network parameters, which is the same as for approximating a single multiplication operation between two real numbers up to a constant multiple.

Similarly, weight sharing is crucial for approximating the second map in (17). Since the function  $g$  are approximated for  $m^D$  instances, weight-sharing networks help reduce the number of distinct network parameters, see Figure 4 for an illustration. The number of parameters required for a single evaluation of  $g$  with an approximation error of  $m^{-\beta/d}$  depends on the structure of  $g$ . In our case,  $O(m)$  parameters (up to a poly-logarithmic factor) are sufficient, due to the factorization property of  $p_0$ .

By combining the results above, we can construct weight-sharing neural networks with  $O(m)$  distinct parameters (up to a poly-logarithmic factor) to approximate (15) with an error of  $m^{-\beta/d}$ .

Returning to the problem of approximating (14), a key difference between (14) and (15) lies in the range of the integral, which depends on  $(\mathbf{x}, t)$ . In particular, the diameter of the range also varies with  $t$ . As a result, we must use different quadrature weights and nodes for each pair  $(\mathbf{x}, t)$ . However, these quadrature weights and nodes can be expressed as (very) smooth functions of  $(\mathbf{x}, t)$ , making them easily approximated by deep neural networks. Full proofs, including additional technical details, are provided in the Appendix.

## 6. Sub-Optimality of a Vanilla Score Matching Estimator

One of the main technical difficulties in our results in Section 5 arises from the fact that  $p_t$  is no longer factorizable for  $t > 0$ . In practice, a key component of the success of score-based generative models and diffusion models lies in jointly modeling infinitely many score functions using deep neural networks via the map  $(\mathbf{x}, t) \mapsto \mathbf{f}(\mathbf{x}, t)$  (Song and Ermon, 2019; Song et al., 2021). Note that early works on the score estimation have focused on estimating the single score function  $\mathbf{x} \mapsto \nabla \log p_0(\mathbf{x})$  via the score matching loss

$$\tilde{\ell}_{\mathbf{f}}(\mathbf{x}) = \text{tr}(\nabla \mathbf{f}(\mathbf{x})) + \frac{1}{2} \|\mathbf{f}(\mathbf{x})\|_2^2,$$

which is based on the fact that

$$\frac{1}{2}\mathbb{E}\left[\|\mathbf{f}(\mathbf{X}_0) - \nabla \log p_0(\mathbf{X}_0)\|_2^2\right] = \mathbb{E}\left[\text{tr}(\nabla \mathbf{f}(\mathbf{X}_0)) + \frac{1}{2}\|\mathbf{f}(\mathbf{X}_0)\|_2^2\right] + C$$

under mild assumptions, where  $C$  is a constant depending only on  $p_0$  (Hyvärinen, 2005).

For a given class  $\mathcal{F}$  of score functions, let  $\widehat{\mathbf{f}}_{\text{VS}}$  be the corresponding empirical risk minimizer, that is,

$$\widehat{\mathbf{f}}_{\text{VS}} \in \underset{\mathbf{f} \in \mathcal{F}}{\text{argmin}} \frac{1}{n} \sum_{i=1}^n \left[ \text{tr}(\nabla \mathbf{f}(\mathbf{X}^i)) + \frac{1}{2} \|\mathbf{f}(\mathbf{X}^i)\|_2^2 \right].$$

The corresponding density estimator can be defined via the Langevin diffusion. Specifically, let  $(\mathbf{Z}_t)_{t>0}$  be the solution to the following Langevin equation:

$$d\mathbf{Z}_t = -\nabla \log p_0(\mathbf{Z}_t)dt + \sqrt{2}d\mathbf{B}_t, \quad \mathbf{Z}_0 \sim \mathcal{N}(\mathbf{0}_D, \mathbb{I}_D).$$

Then, under mild assumptions, the distribution of  $\mathbf{Z}_t$  converges to  $p_0$  as  $t \rightarrow \infty$ . The convergence speed can be exponentially fast under certain conditions on  $p_0$ , such as when  $p_0$  satisfies a Poincaré inequality or a log-Sobolev inequality (Bakry et al., 2014). Hence, one can define a density estimator  $\widehat{p}_{\text{VS}}$  as the limit distribution of the Langevin equation, with the true score function replaced by  $\widehat{\mathbf{f}}_{\text{VS}}$ . We refer to  $\widehat{\mathbf{f}}_{\text{VS}}$  and  $\widehat{p}_{\text{VS}}$  as vanilla score matching estimators for the score and density functions.

Note that vanilla score matching estimators are rarely used in modern large-scale generative problems. One reason is that the trace map  $\text{tr}(\nabla \mathbf{f}(\mathbf{x}))$  is computationally challenging to handle in high-dimensional (large  $D$ ) problems, such as image generation tasks. Therefore, one may raise an important question: if the computation of  $\widehat{\mathbf{f}}_{\text{VS}}$  is tractable, would it perform well? More theoretically, one may ask whether  $\widehat{\mathbf{f}}_{\text{VS}}$ , and consequently  $\widehat{p}_{\text{VS}}$ , can achieve the optimal convergence rate.

Our conjecture is that, regardless of the potential minimax optimality of  $\widehat{\mathbf{f}}_{\text{VS}}$ , the estimator  $\widehat{p}_{\text{VS}}$  cannot achieve the optimal convergence rate. The rationale behind this conjecture lies in the nature of estimating the score function. From the well-established results on the minimax optimal convergence rate for estimating the density derivative (Stone, 1982; Singh, 1977; Shen and Ghosal, 2017; Yoo and Ghosal, 2016), under suitable assumptions, one can derive the following lower bound for estimating the score function:

$$\inf_{\widehat{\mathbf{f}}} \sup_{p_0 \in \mathcal{G}(\beta, D, d, K)} \mathbb{E} \left[ \left\| \widehat{\mathbf{f}}(\mathbf{X}_0) - \nabla \log p_0(\mathbf{X}_0) \right\|_2 \right] \gtrsim n^{-\frac{\beta-1}{2\beta+d}}, \quad (18)$$

where the infimum is taken over all estimators and  $\mathcal{G}(\beta, D, d, K)$  denotes the class of  $\beta$ -smooth factorizable densities, defined in (11). Although we do not provide a specific proof in this paper, such a result can be obtained by applying the standard Fano's method. We refer readers to Wibisono et al. (2024) for the case  $\beta = 2$  without factorization structures, and to Tsybakov (2008) and Wainwright (2019) for general lower-bound techniques.

The rate in (18) is a lower bound, which implies that the convergence rate of  $\widehat{\mathbf{f}}_{\text{VS}}$  cannot be faster. The slower rate, compared to Theorem 3, arises from the fact that the score function is only  $(\beta - 1)$ -smooth, which is strictly less smooth than the density. From the

convergence rate of the score function estimator  $\widehat{\mathbf{f}}_{\text{VS}}$ , one can derive the same convergence rate with respect to the total variation for the corresponding density estimator  $\widehat{p}_{\text{VS}}$  via Girsanov’s theorem (Girsanov, 1960; Le Gall, 2016); see also Remark 2.3 of Bogachev et al. (2016). While the rate  $n^{-\frac{\beta-1}{2\beta+d}}$  is optimal for estimating the score function, the optimal rate for density estimation with respect to the total variation is strictly faster. Hence, the optimality of  $\widehat{p}_{\text{VS}}$  is not guaranteed. Although we do not have a formal proof that  $d_{\text{TV}}(\widehat{p}_{\text{VS}}, p_0) \gtrsim n^{-(\beta-1)/(2\beta+d)}$ , we conjecture that this is indeed the case and do not pursue a formal proof in the current paper.

## 7. Numerical Experiments

In this section, we conduct a small-scale simulation study to empirically examine our theoretical findings. The numerical experiments are designed to explore three main questions. First, we aim to assess whether diffusion models can perform reasonably well at small to moderate data scales. Although this question is not directly related to our theoretical analysis, it remains a natural and practically relevant question because diffusion models are typically applied to very high-dimensional settings with a large number of parameters. Second, we investigate whether, when a low-dimensional structure such as factorization is present, diffusion models tend to outperform classical methods such as kernel density estimation (KDE). Conversely, in the absence of such structural assumptions apart from smoothness, we conjecture that diffusion models perform comparably to classical estimators, at least in low-to-moderate dimensions (e.g.,  $D \leq 10$ ). Finally, we explore the potential benefits of sparse weight-sharing neural networks compared to fully connected architectures through these experiments.

Before proceeding further, we note that although our theoretical results provide valuable insights into when diffusion models perform well compared to other methods, there remains a substantial gap between the theoretical estimator and its practical implementations. In practice, the number of nonzero network parameters in diffusion models is typically much larger than the available sample size, and various forms of algorithmic regularization (either explicit or implicit) are employed. Moreover, the U-Net architecture widely used in applications differs significantly from the theoretical weight-sharing architecture considered in this work. Given these discrepancies, it is inherently challenging to design simulation studies whose outcomes align precisely with the theoretical predictions.

### 7.1 Data Set Descriptions

Hereafter, we denote  $\mathbf{X}_0 = (X_1, \dots, X_D)$  as the random vector following the true distribution. Throughout our experiments, we fix the data dimension at  $D = 5$ . We analyze three types of true data distributions characterized by different effective dimensions  $d$ : (1)  $d = 1$ , (2)  $d = 2$ , and (3)  $d = D$ . Each true distribution is specified by its marginal distributions and a dependency structure imposed through a copula. Although not reported here, in addition to the marginal distributions and dependency structures described below, we also experimented with various other marginal and copula densities. We found that the results were qualitatively similar and consistent across these settings.

$$\tilde{p}(x) = \begin{cases} \frac{1}{2} + \frac{1}{4D} - \frac{1}{2D} \sqrt{-\frac{1}{4} - \frac{x}{2}}, & -1 \leq x < -\frac{1}{2}, \\ \frac{1}{2} + \frac{1}{4D} - \frac{1}{2D} \sqrt{\frac{1}{4} + \frac{x}{2}}, & -\frac{1}{2} \leq x < 0, \\ \frac{1}{2} - \frac{1}{4D} + \frac{1}{2D} \sqrt{\frac{1}{4} - \frac{x}{2}}, & 0 \leq x < \frac{1}{2}, \\ \frac{1}{2} - \frac{1}{4D} + \frac{1}{2D} \sqrt{-\frac{1}{4} + \frac{x}{2}}, & \frac{1}{2} \leq x \leq 1. \end{cases}$$

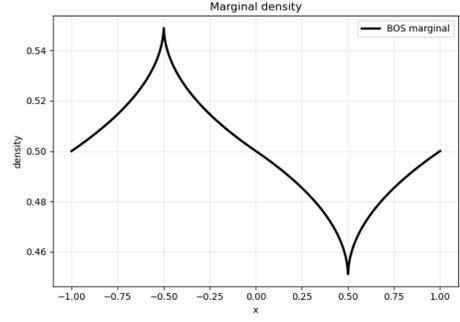


Figure 5: Marginal density used in the experiments.

For the marginal distributions, we consider those used in the experiments of Bos and Schmidt-Hieber (2024), rescaled to lie in the support  $[-1, 1]^D$ . Specifically, each variable  $X_i$  follows a density  $\tilde{p}$ , which belongs to a Hölder class with smoothness  $\beta = 1/2$ . The explicit form of  $\tilde{p}$  is described in Figure 5.

For the dependency structure, we employ three types of copulas: the independence copula ( $d = 1$ ), the Gaussian copula ( $d = 2$ ), and the Clayton copula ( $d = D$ ). For the Gaussian copula, we adopt an AR(1)-type correlation structure with a correlation factor of 0.8. Recall that the Clayton copula is defined as

$$C_\theta(u_1, \dots, u_D) = \left( \sum_{i=1}^D (u_i^{-\theta} - 1) + 1 \right)^{-1/\theta},$$

where  $\theta$  is a parameter controlling the strength of dependence. Its corresponding copula density can be derived in closed form as

$$c_\theta(u_1, \dots, u_D) = \left( \prod_{k=0}^{D-1} (1 + k\theta) \right) \left( \prod_{i=1}^D u_i^{-\theta-1} \right) \left( \sum_{i=1}^D (u_i^{-\theta} - 1) + 1 \right)^{-\frac{1+D\theta}{\theta}}.$$

In our experiments, we set  $\theta = 5$ .

For the training data, we consider sample sizes ranging from  $n = 200$  to  $n = 100,000$ , while the test data consists of 5,000 samples. For each setting, we repeat the experiments five times independently and report the average performance below.

## 7.2 Learning Algorithms and Implementation Details

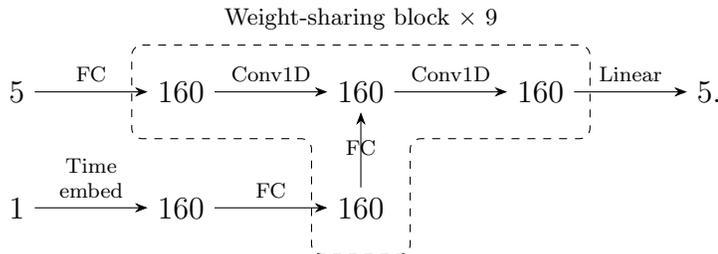
### 7.2.1 DIFFUSION MODELS

We employ the denoising diffusion probabilistic model (DDPM; Ho et al., 2020), which corresponds to the standard OU process and is one of the most widely used diffusion frameworks. The drift coefficient is set as  $\alpha_t = \alpha_{\min} + t(\alpha_{\max} - \alpha_{\min})/(\bar{T} - 1)$  and we fix  $(\alpha_{\min}, \alpha_{\max}, \bar{T}) = (0.0005, 0.01, 500)$  throughout all experiments.

The original DDPM architecture, which contains approximately 37 million parameters, is excessively large for the simulated datasets considered here. To make the comparison computationally feasible, we reduce its size to about 260,000 parameters. In addition, we

modify the architecture, which is originally designed for two-dimensional image inputs, to handle one-dimensional vectors of dimension five. Based on this adjustment, we evaluate two different architectures in our experiments, both constructed to maintain comparable parameter counts (around 260K) to ensure a fair comparison.

- DDPM with weight-sharing neural networks (DDPM with WSNN):** This architecture transforms the 5-dimensional input into a 160-dimensional spatial feature via a fully connected (FC) layer ( $5 \times 160$ ) and embeds the scalar time input into a 160-dimensional time feature, which is further transformed by a FC layer ( $160 \times 160$ ). The spatial feature is then processed by stacking nine weight-sharing blocks while preserving the dimensionality throughout the network. Each block consists of two one-dimensional convolution layers (Conv1D; kernel size 11, padding 5) operating on the spatial feature, with layer normalization. The time feature is transformed by a FC layer ( $160 \times 160$ ) and added to the spatial feature after the first convolution in each block. A residual connection is applied to the spatial feature after the second convolution. The final output is linearly projected back to the 5-dimensional space. With 265,483 parameters, the model follows the pipeline:



- DDPM with fully connected neural networks (DDPM with FCNN):** Unlike the WSNN version, this architecture replaces the Conv1D layers with  $160 \times 160$  FC layers throughout the network. To maintain comparable parameter counts, this architecture repeats the block only three times (instead of nine), resulting in 260,485 parameters.

Regardless of the sample size, both DDPM models are trained using the Adam optimization algorithm (Kingma and Ba, 2015) for 1,000 epochs, with a mini-batch size of 100 and learning rates of  $5 \times 10^{-3}$  for WSNN and  $10^{-3}$  for FCNN. All experiments are implemented in the PyTorch framework and executed on four NVIDIA RTX 3090 GPUs.

### 7.2.2 OTHER BASELINES

As baseline approaches, we consider one classical nonparametric method and one deep learning based method. For the classical method, we employ the KDE with a Gaussian kernel. The optimal bandwidth is selected according to Silverman’s rule of thumb (Silverman, 2018). The KDE implementation, including the sampling procedure, is carried out using the Scikit-learn module in Python.

For the deep learning based method, we adopt the approach proposed by Bos and Schmidt-Hieber (2024), hereafter referred to as BOS. This method follows a two-stage procedure: in the first stage, a KDE is constructed using half of the dataset, and in the second stage, a deep neural network is trained to approximate the resulting kernel density function using the remaining data. It is known that the resulting deep learning model achieves a fast convergence rate under a reasonably well-specified true structural density function. In the KDE stage, the Epanechnikov kernel is employed, and the bandwidth is chosen of the form  $C \times (\log n/n)^{1/D}$ , where the constant  $C$  is selected via 5-fold cross-validation. In the supervised learning stage, a FCNN with  $\lceil \log_2(2n) \rceil$  hidden layers is employed, where each layer consists of  $\lceil (2n)^{1/2} \rceil$  nodes and uses ReLU activation functions. For further experimental details, we refer the reader to the official GitHub repository of Bos and Schmidt-Hieber (2024). Using the trained neural network as an estimated density function, we then generate samples via the Metropolis-Hastings algorithm (MH; Metropolis et al., 1953; Hastings, 1970).

### 7.3 Performance Measure

Since computing the total variation distance requires an explicit density estimator, which is not straightforward for diffusion models, we instead assess performance using the Wasserstein-1 distance based on test samples. Specifically, for each method, we independently generate  $m = 5,000$  samples. For KDE, generating samples is straightforward because its density estimator corresponds to a Gaussian mixture. As mentioned earlier, we use the MH algorithm for BOS.

During MH sampling, we reflect proposed samples at the boundaries to ensure they remain in  $[-1, 1]^D$ , since the neural network is only trained on this support. It is well known that computing the Wasserstein-1 distance between two empirical distributions can be formulated as a linear programming problem. To stabilize the computation, we adopt the Sinkhorn algorithm proposed by Cuturi (2013).

### 7.4 Performance Results

For each setting, we vary the training sample size  $n$  from 200 to 100,000 and compare the Wasserstein-1 distances of the two DDPM variants, one using WSNN and the other using FCNN, with those of KDE and BOS. The results are summarized in Figure 6.

Overall, DDPMs outperform KDE for all cases  $d \in \{1, 2, 5\}$ . DDPMs also outperform BOS for  $d = 2$  and  $d = 5$ , while their performance is comparable to that of BOS for  $d = 1$ , and slightly inferior when  $n \leq 2,000$ . This behavior arises because sampling from the BOS model explicitly exploits knowledge of the support of the true density, which leads to a substantial performance advantage over DDPMs and KDE at small sample sizes. The top-right panel of Figure 6 shows that, when support information is used at the sampling stage, the performance gap between BOS and the other methods narrows considerably for small sample sizes.

The remaining panels demonstrate that DDPMs, even without using support information, still exhibit strong performance across all distributions. Remarkably, for all cases, DDPMs with large sample sizes ( $n \geq 20,000$ ) achieve performance comparable to the oracle benchmark, where the MH algorithm is applied using the true density.

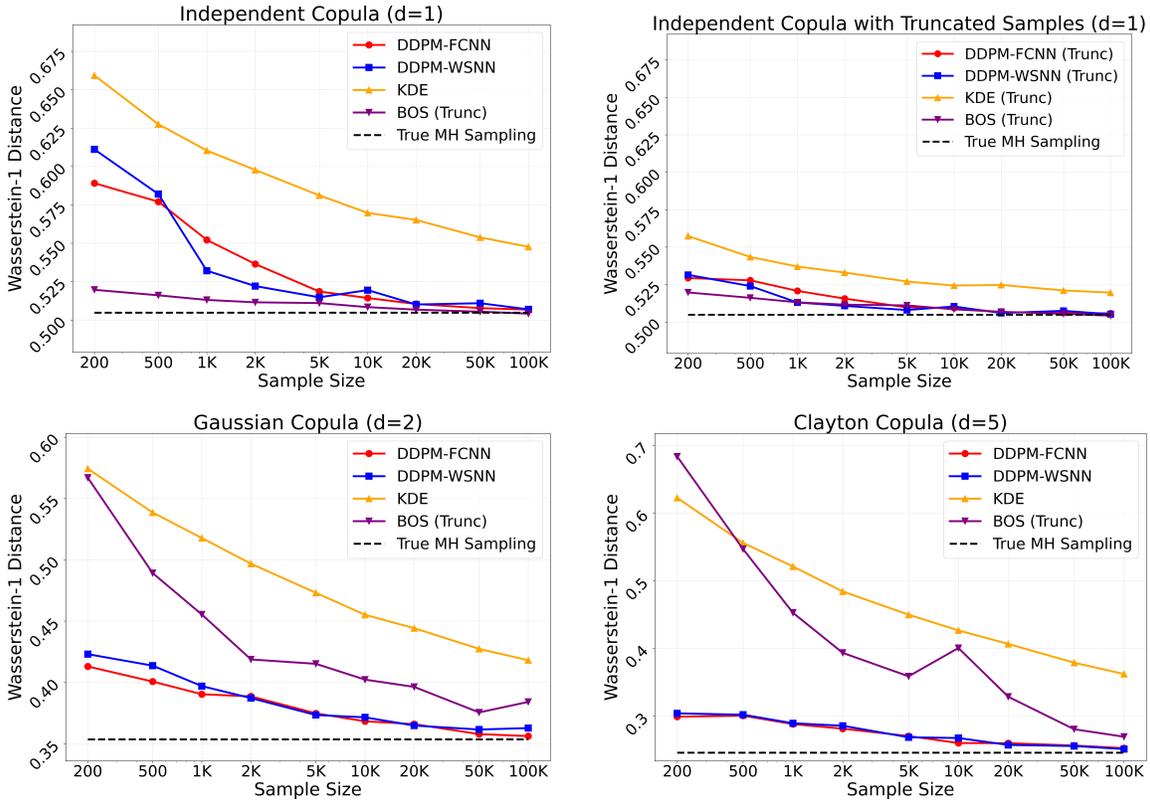


Figure 6: Wasserstein-1 distance values across different copula settings. Top row (left to right): independence copula results without truncation and with truncation for the generated samples. Bottom row (left to right): Gaussian copula and Clayton copula.

Moreover, DDPMs outperform KDE even with a small number of samples, highlighting the empirical effectiveness of diffusion models in limited-data regimes. For  $d = 1$ , DDPMs with  $n = 1,000$  samples already outperform KDE with  $n = 100,000$  samples. Even more strikingly, for  $d = 2$  and  $d = D$ , DDPMs trained with only  $n = 500$  samples outperform KDE trained with  $n = 100,000$  samples.

These findings appear to deviate from our theoretical results, especially when  $d = D$ . After further reflection, our conjecture is as follows: diffusion models may not only adapt to the factorization structure but also to other forms of low-dimensional structure that have not yet been theoretically studied. Even when a density does not exhibit an explicit factorization structure, it may still possess hidden low-dimensional dependencies that diffusion models can effectively capture. Moreover, constructing a distribution completely devoid of any low-dimensional structure is inherently difficult, even in relatively low dimensions (e.g.,  $D = 5$ ).

We emphasize that these observations do not contradict classical nonparametric theory. In practice, estimating a five-dimensional function with 100,000 samples can be more dif-

ficult than estimating a two- or three-dimensional function with only 500 samples, due to the curse of dimensionality.

Furthermore, we conjecture that diffusion models also adapt to non-regular densities, for example, when the Hölder smoothness assumption is violated due to boundary singularities. In our experiments, for  $d = 2$  and  $d = 5$ , the copula density diverges near the boundary, where the variables  $X_1, \dots, X_D$  are highly correlated. Such violations of regularity assumptions may lead to performance degradation for both BOS and KDE, since these methods rely on explicit pointwise estimation of the target density.

Although not shown in the figures, we also observe that DDPMs substantially outperform BOS and KDE when using alternative marginal distributions, including two-component Beta mixture marginals that vanish at the boundary. In this setting, the training of BOS becomes highly unstable and fails to yield performance improvements even for large sample sizes. In contrast, DDPMs consistently outperform BOS and KDE across these settings, providing empirical evidence of their robustness to a wider class of target distributions.

We also note that BOS becomes highly unstable even in moderately high dimensions (e.g.,  $D = 30$ ). This instability arises because BOS directly evaluates the density rather than its logarithm during training, and in high-dimensional settings, the absolute density values become extremely small, leading to numerical underflow. As a result, BOS is not applicable to higher-dimensional cases ( $D > 30$ ).

Finally, across all experiments, the performance of DDPMs with fully connected networks is comparable to that of weight-sharing networks. This observation is consistent with the theoretical results reported in Fan et al. (2025). Nevertheless, it is well known that sparse weight-sharing architectures such as U-Net play a crucial role in achieving state-of-the-art performance in practical applications. We therefore regard a deeper investigation into the theoretical advantages of sparse weight-sharing networks as an important direction for future work.

## 8. Discussion

We have demonstrated that an estimator constructed from the diffusion model is adaptive to the factorization structure and achieves the minimax optimal convergence rates. In this section, we discuss some future directions related to our work.

Firstly, we believe that our analysis can be extended to other performance measures, such as the Wasserstein distance, following the approach of Oko et al. (2023). Also, our analysis can be extended to high-dimensional settings where the data dimension  $D$  diverges as the sample size tends to infinity. In this case, the convergence rate would depend on additional quantities such as  $D$  and  $|\mathcal{I}|$ . An important future task would be to characterize upper bounds for  $D$ , which might depend on the structure of  $p_0$ , to guarantee statistical consistency. Although this generalization is a natural extension for statisticians, the techniques required, such as sharp approximation theory, present significant challenges.

Secondly, while we assumed that  $P_0$  possesses a Lebesgue density, this assumption might be eliminated. For general probability distributions supported on the cube  $[0, 1]^D$ , the minimax optimal rate with respect to the Wasserstein distance is  $n^{-1/D}$  for  $D > 2$ . If we restrict the class to distributions supported on a  $d$ -dimensional space (not necessarily a smooth manifold), the optimal rate improves to  $n^{-1/d}$  (Weed and Bach, 2019). It would be interesting to

investigate whether an estimator constructed from the diffusion model achieves this optimal rate. Further structural assumptions could be considered through conditional independence in directed and undirected graphs, which might replace the factorization assumption  $(\mathbf{F})$  for densities.

Finally, recall that a key component in constructing an optimal estimator is the use of weight-sharing neural networks to approximate functions defined through high-dimensional integrals of the form (15). Recently, physics-informed neural networks (PINNs) have demonstrated remarkable success in modeling solutions to partial differential equations (PDEs) (Karniadakis et al., 2021; Raissi et al., 2019). Notably, many solutions to PDEs, such as the heat equation and the Poisson equation, can be expressed as integrals of the form above (Courant and Hilbert, 2008). This suggests that weight-sharing networks could serve as a promising architecture for theoretical analysis of PINNs.

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**Appendix**

<b>A</b>	<b>Auxiliary Lemmas</b>	<b>36</b>
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**Appendix A. Auxiliary Lemmas**

This section provides auxiliary lemmas for proving the main theorems.

**A.1 Several Bounds Regarding  $p_t(\mathbf{x})$**

In this subsection, we present several lemmas that bound  $p_t(\mathbf{x})$ ,  $\nabla \log p_t(\mathbf{x})$ , and the derivatives of  $p_t(\mathbf{x})$ .

**Lemma 6 (Upper and lower bounds for  $p_t(\mathbf{x})$ )** *Let  $K, \tau_1 > 0$  be given and suppose the true density  $p_0$  satisfies that  $\tau_1 \leq p_0(\mathbf{x}) \leq K$  for any  $\mathbf{x} \in [-1, 1]^D$ . Then, there exists a constant  $C_{S,1} = C_{S,1}(D, K, \tau_1)$  such that*

$$C_{S,1}^{-1} \exp\left(-\frac{D\{(\|\mathbf{x}\|_\infty - \mu_t) \vee 0\}^2}{\sigma_t^2}\right) \leq p_t(\mathbf{x}) \leq C_{S,1} \exp\left(-\frac{\{(\|\mathbf{x}\|_\infty - \mu_t) \vee 0\}^2}{2\sigma_t^2}\right)$$

for every  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 0$ .

**Proof** This is a re-statement of Lemma A.2 in Oko et al. (2023). ■

**Lemma 7 (Boundedness of score function)** *Let  $K, \tau_1 > 0$  be given and suppose the true density  $p_0$  satisfies that  $\tau_1 \leq p_0(\mathbf{x}) \leq K$  for any  $\mathbf{x} \in [-1, 1]^D$ . Then, there exists a positive constant  $C_{S,2} = C_{S,2}(D, K, \tau_1, \bar{\tau}, \underline{\tau})$  such that*

$$\|\nabla \log p_t(\mathbf{x})\|_2 \leq \frac{C_{S,2}}{\sigma_t} \left( \frac{\|\mathbf{x}\|_\infty - \mu_t}{\sigma_t} \vee 1 \right)$$

for every  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 0$ .

**Proof** This is a re-statement of Lemma A.3 in Oko et al. (2023). ■

**Lemma 8 (Boundedness of derivatives)** *Let  $K > 0$  be given and suppose the true density  $p_0$  satisfies that  $p_0(\mathbf{x}) \leq K$  for any  $\mathbf{x} \in [-1, 1]^D$ . For any  $\mathbf{k} \in \mathbb{Z}_{\geq 0}^D$ , there exists a positive constant  $C_{S,3} = C_{S,3}(D, K, \mathbf{k}, \bar{\tau}, \underline{\tau})$  such that*

$$\left| (\mathbf{D}^{\mathbf{k}} p_t)(\mathbf{x}) \right| \leq \frac{C_{S,3}}{\sigma_t^k}$$

for every  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 0$ .

**Proof** This is a re-statement of Lemma A.3 in Oko et al. (2023), where  $k. = \|\mathbf{k}\|_1$ . ■

## A.2 Basic Approximation Results for Neural Networks

In this subsection, we present fundamental approximation results for using ReLU networks to approximate elementary functions. We also define the concatenation and parallelization in weight-sharing networks; see Lemma 13.

**Lemma 9 (Concatenation)** *Let  $K \in \mathbb{N}, \{d_1, \dots, d_{K+1}\} \subseteq \mathbb{N}$  be given. Consider  $L^{(k)} \in \mathbb{N}_{\geq 2}, s^{(k)}, M^{(k)} > 0$  and  $\mathbf{d}^{(k)} = (d_1^{(k)}, \dots, d_{L^{(k)}}^{(k)})^\top \in \mathbb{N}^{L^{(k)}}$  with  $d_1^{(k)} = d_k$  and  $d_{L^{(k)}}^{(k)} = d_{k+1}$  for  $k \in [K]$ . For any neural networks  $f_1, \dots, f_K$  with  $f_k \in \mathcal{F}_{\text{NN}}(L^{(k)}, \mathbf{d}^{(k)}, s^{(k)}, M^{(k)})$ ,  $k \in [K]$ , there exists a neural network  $f \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with*

$$L = \sum_{k=1}^K L^{(k)}, \quad \|\mathbf{d}\|_\infty \leq 2 \max_{k \in [K]} \|\mathbf{d}^{(k)}\|_\infty, \quad s \leq 2 \sum_{k=1}^K s^{(k)}, \quad M = \max_{k \in [K]} M^{(k)}$$

such that  $f(\mathbf{x}) = (f_K \circ \dots \circ f_1)(\mathbf{x})$  for any  $\mathbf{x} \in \mathbb{R}^{d_1}$ .

**Proof** This is a re-statement of Remark 13 in Nakada and Imaizumi (2020). ■

**Lemma 10 (Parallelization)** *Let  $K \in \mathbb{N}$  be given. Consider  $L^{(k)} \in \mathbb{N}_{\geq 2}$ ,  $s^{(k)}, M^{(k)} > 0$ ,  $\mathbf{d}^{(k)} = (d_1^{(k)}, \dots, d_{L^{(k)}}^{(k)})^\top \in \mathbb{N}^{L^{(k)}}$  for  $k \in [K]$ . For any neural networks  $f_1, \dots, f_K$  with*

$$f_k \in \mathcal{F}_{\text{NN}}(L^{(k)}, \mathbf{d}^{(k)}, s^{(k)}, M^{(k)}), \quad k \in [K],$$

*there exists a neural network  $f \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with*

$$\begin{aligned} L &= \max_{k \in [K]} L^{(k)}, \quad \|\mathbf{d}\|_\infty \leq 2 \sum_{k=1}^K \|\mathbf{d}^{(k)}\|_\infty, \\ s &\leq 2 \sum_{k=1}^K \left( s^{(k)} + L d_{L^{(k)}}^{(k)} \right), \quad M \leq \left( \max_{k \in [K]} M^{(k)} \right) \vee 1 \end{aligned}$$

*such that*

$$f(\mathbf{x}) = \left( f_1(\mathbf{x}^{(1)}), \dots, f_K(\mathbf{x}^{(K)}) \right) \in \mathbb{R}^{d_{L^{(1)}}^{(1)} + \dots + d_{L^{(K)}}^{(K)}}$$

*for  $\mathbf{x} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(K)}) \in \mathbb{R}^{d_1^{(1)} + \dots + d_1^{(K)}}$ . If  $L^{(1)} = \dots = L^{(K)} = \tilde{L}$  with  $\tilde{L} \in \mathbb{N}_{\geq 2}$ ,  $(L, \mathbf{d}, s, M)$  also satisfies*

$$L = \tilde{L}, \quad \|\mathbf{d}\|_\infty \leq \sum_{k=1}^K \|\mathbf{d}^{(k)}\|_\infty, \quad s \leq \sum_{k=1}^K s^{(k)}, \quad M \leq \max_{k \in [K]} M^{(k)}.$$

**Proof** This is a re-statement of Lemma F.3 in Oko et al. (2023). ■

**Lemma 11 (Linear function)** *Let  $W \in \mathbb{R}^{d_2 \times d_1}$ ,  $\mathbf{b} \in \mathbb{R}^{d_2}$  be given with  $d_1, d_2 \in \mathbb{N}$ . There exists a neural network  $f_{\text{lin}} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with*

$$L = 2, \quad \mathbf{d} = (d_1, 2d_2, d_2)^\top, \quad s = 2\|W\|_0 + 2\|\mathbf{b}\|_0 + 2d_2, \quad M = \max\{\|W\|_\infty, \|\mathbf{b}\|_\infty, 1\}$$

*such that  $f_{\text{lin}}(\mathbf{x}) = W\mathbf{x} + \mathbf{b}$  for any  $\mathbf{x} \in \mathbb{R}^{d_1}$ .*

**Proof** Note that  $W\mathbf{x} + \mathbf{b} = \rho(W\mathbf{x} + \mathbf{b}) - \rho(-W\mathbf{x} - \mathbf{b})$  for any  $\mathbf{x} \in \mathbb{R}^{d_1}$ . Let  $f_{\text{lin}}(\cdot) = W_2 \rho(W_1 \cdot + \mathbf{b}_1) + \mathbf{b}_2$  with

$$\begin{aligned} W_1 &= \left( W^\top, -W^\top \right)^\top \in \mathbb{R}^{2d_2 \times d_1}, \quad \mathbf{b}_1 = \left( \mathbf{b}^\top, -\mathbf{b}^\top \right)^\top \in \mathbb{R}^{2d_2}, \\ W_2 &= (\mathbb{I}_{d_2}, -\mathbb{I}_{d_2}) \in \mathbb{R}^{d_2 \times 2d_2}, \quad \mathbf{b}_2 = \mathbf{0}_{d_2} \in \mathbb{R}^{d_2}, \end{aligned}$$

where  $\mathbb{I}_{d_2}$  denotes the  $d_2 \times d_2$  identity matrix. Then, the assertion is followed by a simple calculation. ■

**Lemma 12 (Identity function)** For any  $L \geq \mathbb{N}_{\geq 2}$  and  $m \in \mathbb{N}$ , there exists a neural network  $f_{\text{id}}^{(m,L)} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with

$$\mathbf{d} = (m, 2m, \dots, 2m, m)^\top, \quad s = 2mL, \quad M = 1$$

such that  $f_{\text{id}}^{(m,L)}(\mathbf{x}) = \mathbf{x}$  for any  $\mathbf{x} \in \mathbb{R}^m$ .

**Proof** This is a re-statement of Lemma F.2 in Oko et al. (2023). ■

The following lemma provides the concatenation and parallelization of two neural networks, where only one network has shared weight.

**Lemma 13 (Concatenation and parallelization of weight-sharing networks)** Consider the class of weight-sharing networks  $\mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  and vanilla feedforward neural networks  $\mathcal{F}_{\text{NN}}(\tilde{L}, \tilde{\mathbf{d}}, \tilde{s}, \tilde{M})$ . For any neural networks  $f \in \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  and  $\tilde{f} \in \mathcal{F}_{\text{NN}}(\tilde{L}, \tilde{\mathbf{d}}, \tilde{s}, \tilde{M})$ , there exists a neural network  $f_{\text{cc}} \in \mathcal{F}_{\text{WSNN}}(L_{\text{cc}}, \mathbf{d}_{\text{cc}}, s_{\text{cc}}, M_{\text{cc}}, \mathbf{m}_{\text{cc}}, \mathcal{P}_{\text{cc}})$  with

$$L_{\text{cc}} = L + \tilde{L}, \quad \|\mathbf{d}_{\text{cc}}\|_{\infty} \leq 2(\|\mathbf{d}\|_{\infty} \vee \|\tilde{\mathbf{d}}\|_{\infty}), \quad s_{\text{cc}} \leq 2s + 2\tilde{s}, \quad M_{\text{cc}} = M \vee \tilde{M},$$

$\|\mathbf{m}_{\text{cc}}\|_{\infty} = \|\mathbf{m}\|_{\infty}$  and the set of permutation matrices  $\mathcal{P}_{\text{cc}}$  such that  $f_{\text{cc}}(\mathbf{x}) = (\tilde{f} \circ f)(\mathbf{x})$  for any  $\mathbf{x} \in \mathbb{R}^{d_1}$ . Also, there exists a neural network  $f_{\text{pr}} \in \mathcal{F}_{\text{NN}}(L_{\text{pr}}, \mathbf{d}_{\text{pr}}, s_{\text{pr}}, M_{\text{pr}}, \mathbf{m}_{\text{pr}}, \mathcal{P}_{\text{pr}})$  with

$$\begin{aligned} L_{\text{pr}} &= L \vee \tilde{L}, \quad \|\mathbf{d}_{\text{pr}}\|_{\infty} \leq 2\|\mathbf{d}\|_{\infty} + 2\|\tilde{\mathbf{d}}\|_{\infty}, \\ s_{\text{pr}} &\leq 2s + 2\tilde{s} + 2(L \vee \tilde{L})(d_L + \tilde{d}_{\tilde{L}}), \quad M_{\text{pr}} = \max(M, \tilde{M}, 1), \end{aligned}$$

$\|\mathbf{m}_{\text{pr}}\|_{\infty} = \|\mathbf{m}\|_{\infty}$  and the set of permutation matrices  $\mathcal{P}_{\text{pr}}$  such that

$$f_{\text{pr}}(\mathbf{x}) = \left( f(\mathbf{x}_1), \tilde{f}(\mathbf{x}_2) \right) \in \mathbb{R}^{d_L + \tilde{d}_{\tilde{L}}}$$

for any  $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \in \mathbb{R}^{d_1 + \tilde{d}_1}$ .

**Proof** The first assertion can be easily derived from Remark 13 of Nakada and Imaizumi (2020) with

$$\mathbf{m}_{\text{cc}} = (\mathbf{m}, 1, \dots, 1) \in \mathbb{N}^{L_{\text{cc}}-1} \quad \text{and} \quad \mathcal{P}_{\text{cc}} = \mathcal{P} \cup \{\mathcal{Q}_l, \mathcal{R}_l\}_{l \in \{L, \dots, L_{\text{cc}}-1\}},$$

where  $\mathcal{Q}_l$  and  $\mathcal{R}_l$  are the set of  $d_l \times d_l$  and  $d_{l+1} \times d_{l+1}$  identity matrix, respectively.

For the second part, let  $\{W_l, \mathbf{b}_l\}_{l \in [L]}$  and  $\{\tilde{W}_l, \tilde{\mathbf{b}}_l\}_{l \in [\tilde{L}]}$  be the parameter matrices of  $f$  and  $\tilde{f}$ , respectively. If  $L = \tilde{L}$ , let  $\tilde{\mathbf{d}}_{\text{pr}} = (d_1 + \tilde{d}_1, \dots, d_{L+1} + \tilde{d}_{L+1})$  and  $\mathbf{m}_{\text{pr}} = \mathbf{m}$ . Also, for each  $l \in [L]$ , let  $\mathcal{Q}_{\text{pr},l}$  and  $\mathcal{R}_{\text{pr},l}$  be the set of permutation matrices of the form

$$\begin{pmatrix} Q_l^{(j)} & \mathbf{0} \\ \mathbf{0} & \mathbb{I}_{\tilde{d}_l} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} R_l^{(j)} & \mathbf{0} \\ \mathbf{0} & \mathbb{I}_{\tilde{d}_{l+1}} \end{pmatrix}$$

with  $j \in [m_l]$ , respectively. Then, the assertion follows with

$$W_{\text{pr},l} = \begin{pmatrix} W_l & \mathbf{0} \\ \mathbf{0} & m_l^{-1} \widetilde{W}_l \end{pmatrix} \quad \text{and} \quad \mathbf{b}_{\text{pr},l} = \begin{pmatrix} \mathbf{b}_l \\ m_l^{-1} \widetilde{\mathbf{b}}_l \end{pmatrix}, \quad l \in [L-1],$$

and  $\mathcal{P}_{\text{pr}} = \{\mathcal{Q}_{\text{pr},l}, \mathcal{R}_{\text{pr},l}\}_{l \in [L-1]}$ , where  $\{W_{\text{pr},l}, \mathbf{b}_{\text{pr},l}\}_{l \in [L]}$  are the parameter matrices of  $f_{\text{pr}}$ . If  $L = \widetilde{L} + 1$ , consider a neural network  $\bar{\mathbf{f}}$  with  $L$ -layer and parameter matrices  $\{\overline{W}_l, \overline{\mathbf{b}}_l\}_{l \in [L]}$ , where  $\overline{W}_l = \widetilde{W}_l, \overline{\mathbf{b}}_l = \widetilde{\mathbf{b}}_l$  for  $l \in [\widetilde{L} - 1]$ , and

$$\overline{W}_{\widetilde{L}} = \begin{pmatrix} \widetilde{W}_{\widetilde{L}} \\ -\widetilde{W}_{\widetilde{L}} \end{pmatrix}, \quad \overline{\mathbf{b}}_{\widetilde{L}} = \begin{pmatrix} \widetilde{\mathbf{b}}_{\widetilde{L}} \\ -\widetilde{\mathbf{b}}_{\widetilde{L}} \end{pmatrix}, \quad \overline{W}_{\widetilde{L}+1} = \begin{pmatrix} \mathbb{I}_{\widetilde{d}_{\widetilde{L}+1}} \\ -\mathbb{I}_{\widetilde{d}_{\widetilde{L}+1}} \end{pmatrix}, \quad \overline{\mathbf{b}}_{\widetilde{L}+1} = \mathbf{0}_{2\widetilde{d}_{\widetilde{L}+1}}.$$

We then apply the results for the case of parallelization between same layer network. If  $L > \widetilde{L} + 1$ , consider a weight-sharing neural network  $\bar{\mathbf{f}} = \mathbf{f}_{\text{id}}^{(\widetilde{d}_{\widetilde{L}+1}, L - \widetilde{L})} \circ \widetilde{\mathbf{f}}$  with  $L$ -layer, where  $\mathbf{f}_{\text{id}}^{(\widetilde{d}_{\widetilde{L}+1}, L - \widetilde{L})}$  is the neural network in Lemma 12. We then apply the results for the case of parallelization between same layer network.

If  $L = \widetilde{L} - 1$ , consider a weight-sharing neural network  $\bar{\mathbf{f}}$  with  $\widetilde{L}$ -layer, parameter matrices  $\{\overline{W}_l, \overline{\mathbf{b}}_l\}_{l \in [\widetilde{L}]}$  with  $\overline{W}_l = W_l, \overline{\mathbf{b}}_l = \mathbf{b}_l$  for  $l \in [L - 1]$ , and

$$\overline{W}_L = \begin{pmatrix} W_L \\ -W_L \end{pmatrix}, \quad \overline{\mathbf{b}}_L = \begin{pmatrix} \mathbf{b}_L \\ -\mathbf{b}_L \end{pmatrix}, \quad \overline{W}_{L+1} = \begin{pmatrix} \mathbb{I}_{d_{L+1}} \\ -\mathbb{I}_{d_{L+1}} \end{pmatrix}, \quad \overline{\mathbf{b}}_{L+1} = \mathbf{0}_{2d_{L+1}},$$

$m_L = 1$  and the set of permutation matrices  $\mathcal{P} \cup \{\mathcal{Q}_L, \mathcal{R}_L\}$ , where  $\mathcal{Q}_L$  and  $\mathcal{R}_L$  are the set of  $d_L \times d_L$  and  $2d_{L+1} \times 2d_{L+1}$  identity matrix, respectively. We then apply the results for the case of parallelization between same layer network. If  $L < \widetilde{L} - 1$ , consider a weight-sharing neural network  $\bar{\mathbf{f}} = \mathbf{f}_{\text{id}}^{(d_{L+1}, \widetilde{L} - L)} \circ \widetilde{\mathbf{f}}$  with  $\widetilde{L}$ -layer and the set of permutation matrices  $\mathcal{P} \cup \{\mathcal{Q}_l, \mathcal{R}_l\}_{L \leq l \leq \widetilde{L} - 1}$ , where  $\mathbf{f}_{\text{id}}^{(d_{L+1}, \widetilde{L} - L)}$  is the neural network in Lemma 12 and for each  $l \in \{L, \dots, \widetilde{L} - 1\}$ ,  $\mathcal{Q}_l$  and  $\mathcal{R}_l$  are the set of  $d_l \times d_l$  and  $d_{l+1} \times d_{l+1}$  identity matrix, respectively. We then apply the results for the case of parallelization between same layer network. ■

**Lemma 14 (Multiplication)** *Let  $m \geq 2, C \geq 1, 0 < \tilde{\epsilon} \leq 1$  be given. For any  $\epsilon > 0$ , there exists a positive constant  $C_{N,1}$  and a neural network  $f_{\text{mult}} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with*

$$L \leq C_{N,1} \log m \{\log(1/\epsilon) + m \log C\}, \quad \mathbf{d} = (m, 48m, \dots, 48m, 1)^\top, \\ s \leq C_{N,1} m \{\log(1/\epsilon) + \log C\}, \quad M = C^m$$

such that

$$\left| f_{\text{mult}}(\tilde{\mathbf{x}}) - \prod_{i=1}^m x_i \right| \leq \epsilon + mC^{m-1}\tilde{\epsilon}, \quad \forall \mathbf{x} \in [-C, C]^m, \tilde{\mathbf{x}} \in \mathbb{R}^m \text{ with } \|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon},$$

$\|f_{\text{mult}}\|_\infty \leq C^m$  and  $f_{\text{mult}}(\tilde{\mathbf{x}}) = 0$  if  $0 \in \{\tilde{x}_1, \dots, \tilde{x}_m\}$ .

**Proof** This is a re-statement of Lemma F.6 in Oko et al. (2023). ■

**Lemma 15 (Clipping function)** Let  $\mathbf{b} = (\underline{b}_1, \dots, \underline{b}_m)$ ,  $\bar{\mathbf{b}} = (\bar{b}_1, \dots, \bar{b}_m) \in \mathbb{R}^m$  be given with  $m \in \mathbb{N}$  and  $\underline{b}_i \leq \bar{b}_i$  for all  $i \in [m]$ . Then, there exists a neural network

$$f_{\text{clip}}^{(\mathbf{b}, \bar{\mathbf{b}})} \in \mathcal{F}_{\text{NN}}(2, (m, 2m, m)^\top, 7m, \|\mathbf{b}\|_\infty \vee \|\bar{\mathbf{b}}\|_\infty)$$

such that

$$f_{\text{clip}}^{(\mathbf{b}, \bar{\mathbf{b}})}(\mathbf{x}) = (\bar{b}_1 \wedge \{x_1 \vee \underline{b}_1\}, \dots, \bar{b}_m \wedge \{x_m \vee \underline{b}_m\}) \in \mathbb{R}^m$$

for  $\mathbf{x} = (x_1, \dots, x_m) \in \mathbb{R}^m$ .

**Proof** This is a re-statement of Lemma F.4 in Oko et al. (2023). ■

**Lemma 16 (Logarithm function)** For any  $0 < \epsilon < 1/4$ , there exists a positive constant  $C_{N,2}$  and a neural network  $f_{\log} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with

$$\begin{aligned} L &\leq C_{N,2} \{\log(1/\epsilon)\}^2 \log \log(1/\epsilon), & \|\mathbf{d}\|_\infty &\leq C_{N,2} \{\log(1/\epsilon)\}^3 \\ s &\leq C_{N,2} \{\log(1/\epsilon)\}^5 \log \log(1/\epsilon), & M &\leq \exp(8\{\log(1/\epsilon)\}^2) \end{aligned}$$

such that

$$|\log x - f_{\log}(\tilde{x})| \leq \epsilon + \frac{|x - \tilde{x}|}{\epsilon}$$

for  $x \in [\epsilon, 1/\epsilon]$  and  $\tilde{x} \in \mathbb{R}$ .

**Proof** Let  $0 < \epsilon < 1/4$ ,  $\delta = 1/8$  and  $D_1 = \lfloor \frac{2\log(1/\epsilon)}{\log(1+\delta)} - 1 \rfloor + 1$ . Then,  $[\epsilon, 1/\epsilon] \subseteq \bigcup_{i=1}^{D_1} [\underline{T}_i, \bar{T}_i]$ , where  $\underline{T}_i = (1+\delta)^{i-1}\epsilon$  and  $\bar{T}_i = (1+\delta)^{i+1}\epsilon$  for  $i \in [D_1]$ . Let  $D_2 = \lfloor \frac{\log(1/\epsilon)}{\log 2} \rfloor + 3$ . For any  $i \in [D_1]$  and  $x \in [\underline{T}_i, \bar{T}_i]$ , Taylor's theorem yields that

$$\log x = P_i(x) + \frac{(-1)^{D_2-1} (x - \underline{T}_i)^{D_2}}{D_2 \{\underline{T}_i + \xi(\bar{T}_i - \underline{T}_i)\}^{D_2}}$$

for a suitable  $\xi \in [0, 1]$ , where

$$P_i(x) = \log \underline{T}_i + \frac{x - \underline{T}_i}{\underline{T}_i} + \sum_{k=2}^{D_2-1} \frac{(-1)^{k-1} (x - \underline{T}_i)^k}{k \underline{T}_i^k}.$$

Since  $x - \underline{T}_i \leq \bar{T}_i - \underline{T}_i = \underline{T}_i(\delta^2 + 2\delta)$  and  $\underline{T}_i \leq \underline{T}_i + \xi(\bar{T}_i - \underline{T}_i)$ , it follows that

$$|\log x - P_i(x)| \leq \frac{1}{D_2} \left( \frac{\bar{T}_i - \underline{T}_i}{\underline{T}_i} \right)^{D_2} = \frac{(\delta^2 + 2\delta)^{D_2}}{D_2} \leq \frac{2^{-D_2}}{D_2} \leq \frac{\epsilon}{D_2}, \quad i \in [D_1] \quad (19)$$

for  $x \in [\underline{T}_i, \overline{T}_i]$ . Let  $N_1$  be a constant in Lemma 14. For  $k \geq 2$ , there exists a neural network  $f_{\text{mult}}^{(k)} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}^{(k)}, \mathbf{d}_{\text{mult}}^{(k)}, s_{\text{mult}}^{(k)}, M_{\text{mult}}^{(k)})$  with

$$\begin{aligned} L_{\text{mult}}^{(k)} &\leq N_1(k + D_2) \log k \{\log(1/\epsilon) + \log D_2\}, & \mathbf{d}_{\text{mult}}^{(k)} &= (k, 48k, \dots, 48k, 1)^\top, \\ s_{\text{mult}}^{(k)} &\leq N_1 k(k + D_2) \{\log(1/\epsilon) + \log D_2\}, & M_{\text{mult}}^{(k)} &= \epsilon^{-k} \end{aligned} \quad (20)$$

such that  $|f_{\text{mult}}^{(k)}(x_1, \dots, x_k) - \prod_{i=1}^k x_i| \leq \epsilon^{D_2}/D_2$  for any  $x_1, \dots, x_k \in [-\epsilon^{-1}, \epsilon^{-1}]$ . For any  $k \geq 1$  and  $i \in [D_1]$ , Lemma 11 implies that there exists a neural network  $f_{\text{lin}}^{(i,k)} \in \mathcal{F}_{\text{NN}}(2, (1, 2k, k)^\top, 6k, \underline{T}_i)$  such that  $f_{\text{lin}}^{(i,k)}(x) = (x - \underline{T}_i, \dots, x - \underline{T}_i)^\top \in \mathbb{R}^k$  for any  $x \in \mathbb{R}$ . Combining Lemma 9 with the last display, it follows that  $f_{\text{pow}}^{(i,k)} = f_{\text{mult}}^{(k)} \circ f_{\text{lin}}^{(i,k)} \in \mathcal{F}_{\text{NN}}(L_{\text{pow}}^{(i,k)}, \mathbf{d}_{\text{pow}}^{(i,k)}, s_{\text{pow}}^{(i,k)}, M_{\text{pow}}^{(i,k)})$  for  $i \in [D_1], k \geq 2$  with

$$L_{\text{pow}}^{(i,k)} = L_{\text{mult}}^{(k)} + 2, \quad \|\mathbf{d}_{\text{pow}}^{(i,k)}\|_\infty \leq 96k, \quad s_{\text{pow}}^{(i,k)} = 2s_{\text{mult}}^{(k)} + 12k, \quad M_{\text{pow}}^{(i,k)} = \underline{T}_i \vee M_{\text{mult}}^{(k)}$$

and

$$\left| f_{\text{pow}}^{(i,k)}(x) - (x - \underline{T}_i)^k \right| \leq \frac{\epsilon^{D_2}}{D_2},$$

for  $x \in [\epsilon, \epsilon^{-1}]$ . Consider functions  $f_1, \dots, f_{D_1} : \mathbb{R} \rightarrow \mathbb{R}$  such that

$$f_i(\cdot) = \log \underline{T}_i + \frac{f_{\text{lin}}^{(i,1)}(\cdot)}{\underline{T}_i} + \sum_{k=2}^{D_2-1} \frac{(-1)^{k-1} f_{\text{pow}}^{(i,k)}(\cdot)}{k \underline{T}_i^k}, \quad i \in [D_1].$$

Since  $f_i - \log \underline{T}_i$  is a linear combination of  $f_{\text{lin}}^{(i,1)}, f_{\text{pow}}^{(i,2)}, \dots, f_{\text{pow}}^{(i,D_2-1)}$  for  $i \in [D_1]$ , Lemma 9, Lemma 10 and Lemma 11 implies that  $f_i \in \mathcal{F}_{\text{NN}}(L^{(i)}, \mathbf{d}^{(i)}, s^{(i)}, M^{(i)})$  with

$$\begin{aligned} L^{(i)} &\leq L_{\text{pow}}^{(i,D_2-1)} + 2 \leq D_3 D_2 \log D_2 \{\log(1/\epsilon) + \log D_2\}, \\ \|\mathbf{d}^{(i)}\|_\infty &\leq 2 \max \left( 2 \sum_{k=2}^{D_2-1} \|\mathbf{d}_{\text{pow}}^{(i,k)}\|_\infty + 4, D_2 - 1 \right) \leq D_3 D_2^2, \\ s^{(i)} &\leq 2 \left\{ \sum_{k=2}^{D_2-1} \left( s_{\text{pow}}^{(i,k)} + L_{\text{pow}}^{(i,D_2-1)} + 2 \right) + L_{\text{pow}}^{(i,D_2-1)} + 8 \right\} + 2D_2 + 2 \\ &\leq D_3 D_2^3 \log D_2 \{\log(1/\epsilon) + \log D_2\}, \\ M^{(i)} &\leq \left( \max_{k \in [D_2-1]} M_{\text{pow}}^{(i,k)} \right) \vee \underline{T}_i^{-D_2+1} \leq \epsilon^{-D_2} \end{aligned} \quad (21)$$

for a large enough constant  $D_3 = D_3(N_1)$ . Then,

$$\begin{aligned} |P_i(x) - f_i(x)| &\leq \sum_{k=2}^{D_2-1} \frac{|f_{\text{pow}}^{(i,k)}(x) - (x - \underline{T}_i)^k|}{k \underline{T}_i^k} \\ &\leq \frac{D_2 - 2}{2\epsilon^{D_2-1}} \max_{2 \leq k \leq D_2-1} \left| f_{\text{pow}}^{(i,k)}(x) - (x - \underline{T}_i)^k \right| \leq \frac{\epsilon}{2}, \quad i \in [D_1] \end{aligned}$$

for  $x \in [\epsilon, \epsilon^{-1}]$ , where the first inequality holds because  $\underline{T}_i \geq \epsilon$ . Combining (19) with the last display, we have

$$|\log x - f_i(x)| \leq \left( \frac{1}{2} + \frac{1}{D_2} \right) \epsilon, \quad i \in [D_1] \quad (22)$$

for  $x \in [\underline{T}_i, \bar{T}_i]$ . Consider functions  $f_{\text{swit}}^{(1)}, \dots, f_{\text{swit}}^{(D_1)} : \mathbb{R} \rightarrow [0, 1]$  such that

$$\begin{aligned} f_{\text{swit}}^{(1)}(\cdot) &= \frac{1}{\bar{T}_1 - \underline{T}_2} \rho \left( -f_{\text{clip}}^{(\underline{T}_2, \bar{T}_1)}(\cdot) + \bar{T}_1 \right), \\ f_{\text{swit}}^{(i)}(\cdot) &= \frac{1}{\bar{T}_{i-1} - \underline{T}_i} \rho \left( f_{\text{clip}}^{(\underline{T}_i, \bar{T}_{i-1})}(\cdot) - \underline{T}_i \right) - \frac{1}{\bar{T}_i - \underline{T}_{i+1}} \rho \left( f_{\text{clip}}^{(\underline{T}_{i+1}, \bar{T}_i)}(\cdot) - \underline{T}_{i+1} \right), \\ f_{\text{swit}}^{(D_1)}(\cdot) &= \frac{1}{\bar{T}_{D_1-1} - \underline{T}_{D_1}} \rho \left( f_{\text{clip}}^{(\underline{T}_{D_1}, \bar{T}_{D_1-1})}(\cdot) - \underline{T}_{D_1} \right), \quad 2 \leq i \leq D_1 - 1, \end{aligned}$$

where  $f_{\text{clip}}^{(\underline{T}_i, \bar{T}_{i-1})} \in \mathcal{F}_{\text{NN}}(2, (1, 2, 1)^\top, 7, 8\epsilon^{-1})$  denotes the neural network in Lemma 15. Note that  $\sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) = 1$  for  $x \in \mathbb{R}$  and  $f_{\text{swit}}^{(i)}(x) = 0$  for  $x \in \bigcup_{j=1}^{D_1} [\underline{T}_j, \bar{T}_j] \setminus [\underline{T}_i, \bar{T}_i]$ ,  $i \in [D_1]$ . Consider a function  $f : \mathbb{R} \rightarrow \mathbb{R}$  such that  $f(\cdot) = \sum_{i=1}^{D_1} f_{\text{mult}}^{(2)}(f_{\text{swit}}^{(i)}(\cdot), f_i(\cdot))$ . Since  $|f_{\text{mult}}^{(2)}(x_1, x_2) - x_1 x_2| \leq \epsilon^{D_2}/D_2$  for any  $x_1, x_2 \in [-\epsilon^{-1}, \epsilon^{-1}]$ , we have

$$\begin{aligned} |\log x - f(x)| &\leq \left| \log x - \sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) f_i(x) \right| + \frac{D_1 \epsilon^{D_2}}{D_2} \\ &= \left| \sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) \{ \log x - f_i(x) \} \right| + \frac{D_1 \epsilon^{D_2}}{D_2} \\ &\leq \sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) |\log x - f_i(x)| + \frac{D_1 \epsilon^{D_2}}{D_2} \leq \left( \frac{1}{2} + \frac{1}{D_2} \right) \epsilon \sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) + \frac{D_1 \epsilon^{D_2}}{D_2} \\ &= \left( \frac{1}{2} + \frac{1 + D_1 \epsilon^{D_2-1}}{D_2} \right) \epsilon \leq \epsilon \end{aligned}$$

for  $x \in \bigcup_{i=1}^{D_1} [\underline{T}_i, \bar{T}_i]$ , where the second inequality holds by (22). Combining (20) and (21) with Lemma 10 and Lemma 9, we have  $f_{\text{mult}}^{(2)}(f_{\text{swit}}^{(i)}(\cdot), f_i(\cdot)) \in \mathcal{F}_{\text{NN}}(\tilde{L}^{(i)}, \tilde{\mathbf{d}}^{(i)}, \tilde{\mathbf{s}}^{(i)}, \tilde{M}^{(i)})$  for  $i \in [D_1]$  with

$$\begin{aligned} \tilde{L}^{(i)} &\leq (L^{(i)} \vee 2) + L_{\text{mult}}^{(2)} \leq D_4 D_2 \log D_2 \{ \log(1/\epsilon) + \log D_2 \} \\ \|\tilde{\mathbf{d}}^{(i)}\|_\infty &\leq 2 \max \left( 2 \|\mathbf{d}^{(i)}\|_\infty + 4, \|\mathbf{d}_{\text{mult}}^{(2)}\|_\infty \right) \leq D_4 D_2^2 \\ \tilde{\mathbf{s}}^{(i)} &\leq 4s^{(i)} + 4(L^{(i)} \vee 2) + 2s_{\text{mult}}^{(2)} + 28 \leq D_4 D_2^3 \log D_2 \{ \log(1/\epsilon) + \log D_2 \} \\ \tilde{M}^{(i)} &\leq \max \left( 8\epsilon^{-1}, M^{(i)}, M_{\text{mult}}^{(2)}, 1 \right) \leq \epsilon^{-D_2}, \end{aligned}$$

where  $D_4 = D_4(D_3)$  is a large enough constant. Let  $f_{\text{clip}}^{(\epsilon, \epsilon^{-1})} \in \mathcal{F}_{\text{NN}}(2, (1, 2, 1)^\top, 7, \epsilon^{-1})$  be the neural network in Lemma 15. Since  $f$  is a linear combination of  $f_{\text{mult}}^{(2)}(f_{\text{swit}}^{(i)}(\cdot), f_i(\cdot))$  for

each  $i \in [D_1]$ , Lemma 9, Lemma 10 and Lemma 11 implies that  $f \circ f_{\text{clip}}^{(\epsilon, \epsilon^{-1})} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with

$$\begin{aligned} L &\leq \max_{i \in [D_1]} \tilde{L}^{(i)} + 4 \leq D_5 \{\log(1/\epsilon)\}^2 \log \log(1/\epsilon) \\ \|\mathbf{d}\|_\infty &\leq 2 \max \left( 2 \sum_{i=1}^{D_1} \|\tilde{\mathbf{d}}^{(i)}\|_\infty, 4D_1 \right) \leq D_5 \{\log(1/\epsilon)\}^3 \\ s &\leq 2 \sum_{i=1}^{D_1} \left( \tilde{s}^{(i)} + \max_{j \in [D_1]} \tilde{L}^{(j)} \right) + 4D_1 + 18 \leq D_5 \{\log(1/\epsilon)\}^5 \log \log(1/\epsilon) \\ M &\leq \max_{i \in [D_1]} \tilde{M}^{(i)} \vee \epsilon^{-1} \leq \exp(8\{\log(1/\epsilon)\}^2) \end{aligned}$$

for large enough constant  $D_5 = D_5(D_4)$ . Note that  $|(f \circ f_{\text{clip}}^{(\epsilon, \epsilon^{-1})})(\tilde{x}) - \log x| \leq |(f \circ f_{\text{clip}}^{(\epsilon, \epsilon^{-1})})(\tilde{x}) - \log(\epsilon^{-1} \wedge \{\tilde{x} \vee \epsilon\})| + |\log(\epsilon^{-1} \wedge \{\tilde{x} \vee \epsilon\}) - \log x| \leq \epsilon + \epsilon^{-1}|x - \tilde{x}|$  for any  $x \in [\epsilon, \epsilon^{-1}]$  and  $\tilde{x} \in \mathbb{R}$ . Then, the assertion follows by re-defining the constant.  $\blacksquare$

**Lemma 17 (Negative exponential function)** *For any  $0 < \epsilon < 2^{-4e+2}$ , there exists a positive constant  $C_{N,3}$  and a neural network  $f_{\text{exp}} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with*

$$\begin{aligned} L &\leq C_{N,3} \log(1/\epsilon) \log \log(1/\epsilon), \quad \|\mathbf{d}\|_\infty \leq C_{N,3} \{\log(1/\epsilon)\}^3 \\ s &\leq C_{N,3} \{\log(1/\epsilon)\}^4, \quad M \leq C_{N,3} \epsilon^{-1} \end{aligned}$$

such that

$$|e^{-x} - f_{\text{exp}}(\tilde{x})| \leq \epsilon + |x - \tilde{x}|$$

for any  $x \geq 0$  and  $\tilde{x} \in \mathbb{R}$ .

**Proof** Let  $0 < \epsilon < 2^{-4e+2}$ ,  $D_1 = \lfloor \log(4/\epsilon) \rfloor + 1$ ,  $D_2 = \lfloor \log(4/\epsilon) / \log 2 \rfloor + 1$  and  $\underline{T}_i = i - 1$ ,  $\overline{T}_i = i + 1$  for  $i \in [D_1]$ . Then, Taylor's theorem yields that for any  $i \in [D_1]$  and  $x \in [\underline{T}_i, \overline{T}_i]$ ,

$$e^{-x} = e^{-\underline{T}_i} e^{-(x-\underline{T}_i)} = e^{-\underline{T}_i} \left\{ P_i(x) + \frac{(-1)^{D_2} e^{-\xi(x-\underline{T}_i)} (x-\underline{T}_i)^{D_2}}{D_2!} \right\}$$

for a suitable  $\xi \in [0, 1]$ , where

$$P_i(x) = 1 - (x - \underline{T}_i) + \sum_{k=2}^{D_2-1} \frac{(-1)^k (x - \underline{T}_i)^k}{k!}.$$

Since  $0 \leq x - \underline{T}_i \leq 2$  and  $\underline{T}_i \geq 0$ , it follows that

$$|e^{-x} - e^{-\underline{T}_i} P_i(x)| \leq \frac{2^{D_2}}{D_2!} \leq \left( \frac{2e}{D_2} \right)^{D_2} \leq \left( \frac{1}{2} \right)^{D_2} \leq \frac{\epsilon}{4}, \quad (23)$$

where the second inequality holds because  $k! \geq k^k e^{-k}$  for any  $k \in \mathbb{N}$ . Let  $N_1$  be a constant in Lemma 14. For  $k \geq 2$ , there exists a neural network  $f_{\text{mult}}^{(k)} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}^{(k)}, \mathbf{d}_{\text{mult}}^{(k)}, s_{\text{mult}}^{(k)}, M_{\text{mult}}^{(k)})$  with

$$\begin{aligned} L_{\text{mult}}^{(k)} &\leq N_1 \log k \{\log(4D_2/\epsilon^2) + k \log 2\}, & \mathbf{d}_{\text{mult}}^{(k)} &= (k, 48k, \dots, 48k, 1)^\top, \\ s_{\text{mult}}^{(k)} &\leq N_1 k \{\log(4D_2/\epsilon^2) + \log 2\}, & M_{\text{mult}}^{(k)} &= 2^k \end{aligned} \quad (24)$$

such that  $|f_{\text{mult}}^{(k)}(x_1, \dots, x_k) - \prod_{i=1}^k x_i| \leq \epsilon^2/(4D_2)$  for any  $x_1, \dots, x_k \in [-2, 2]$ . For any  $k \geq 1$  and  $i \in [D_1]$ , Lemma 11 implies that there exists a neural network

$$f_{\text{lin}}^{(i,k)} \in \mathcal{F}_{\text{NN}}(2, (1, 2k, k)^\top, 6k, \underline{T}_i)$$

such that  $f_{\text{lin}}^{(i,k)}(x) = (x - \underline{T}_i, \dots, x - \underline{T}_i)^\top \in \mathbb{R}^k$  for any  $x \in \mathbb{R}$ . Combining Lemma 9 with the last display, it follows that  $f_{\text{pow}}^{(i,k)} = f_{\text{mult}}^{(k)} \circ f_{\text{lin}}^{(i,k)} \in \mathcal{F}_{\text{NN}}(L_{\text{pow}}^{(i,k)}, \mathbf{d}_{\text{pow}}^{(i,k)}, s_{\text{pow}}^{(i,k)}, M_{\text{pow}}^{(i,k)})$  for  $i \in [D_1], k \geq 2$  with

$$L_{\text{pow}}^{(i,k)} = L_{\text{mult}}^{(k)} + 2, \quad \|\mathbf{d}_{\text{pow}}^{(i,k)}\|_\infty \leq 96k, \quad s_{\text{pow}}^{(i,k)} = 2s_{\text{mult}}^{(k)} + 12k, \quad M_{\text{pow}}^{(i,k)} = \underline{T}_i \vee M_{\text{mult}}^{(k)}$$

and

$$\left| f_{\text{pow}}^{(i,k)}(x) - (x - \underline{T}_i)^k \right| \leq \frac{\epsilon^2}{4D_2}$$

for  $x \in [\underline{T}_i, \bar{T}_i]$ . Consider functions  $f_1, \dots, f_{D_1} : \mathbb{R} \rightarrow \mathbb{R}$  such that

$$f_i(\cdot) = 1 - f_{\text{lin}}^{(i,1)}(\cdot) + \sum_{k=2}^{D_2-1} \frac{(-1)^k f_{\text{pow}}^{(i,k)}(\cdot)}{k!}, \quad i \in [D_1].$$

Since  $f_i - 1$  is a linear combination of  $f_{\text{lin}}^{(i,1)}, f_{\text{pow}}^{(i,2)}, \dots, f_{\text{pow}}^{(i,D_2-1)}$ , Lemma 9, Lemma 10 and Lemma 11 implies that  $f_i \in \mathcal{F}_{\text{NN}}(L^{(i)}, \mathbf{d}^{(i)}, s^{(i)}, M^{(i)})$  with

$$\begin{aligned} L^{(i)} &\leq L_{\text{pow}}^{(i,D_2-1)} + 2 \leq D_3 \log D_2 \{\log(1/\epsilon) + D_2\} \\ \|\mathbf{d}^{(i)}\|_\infty &\leq 2 \max \left( 2 \sum_{k=2}^{D_2-1} \|\mathbf{d}_{\text{pow}}^{(i,k)}\|_\infty + 4, D_2 - 1 \right) \leq D_3 D_2^2 \\ s^{(i)} &\leq 2 \left\{ \sum_{k=2}^{D_2-1} \left( s_{\text{pow}}^{(i,k)} + L_{\text{pow}}^{(i,D_2-1)} + 2 \right) + L_{\text{pow}}^{(i,D_2-1)} + 8 \right\} + 2D_2 + 2 \\ &\leq D_3 D_2^2 \{\log(1/\epsilon) + D_2\} \\ M^{(i)} &\leq \left( \max_{k \in [D_2-1]} M_{\text{pow}}^{(i,k)} \right) \vee 1 \leq (D_1 + 1) \vee 2^{D_2-1} \end{aligned} \quad (25)$$

for a large enough constant  $D_3 = D_3(N_1)$ . Then,

$$\begin{aligned} |P_i(x) - f_i(x)| &\leq \sum_{k=2}^{D_2-1} \frac{|f_{\text{pow}}^{(i,k)}(x) - (x - \underline{T}_i)^k|}{k!} \\ &\leq D_2 \max_{2 \leq k \leq D_2-1} \left| f_{\text{pow}}^{(i,k)}(x) - (x - \underline{T}_i)^k \right| \leq \frac{\epsilon^2}{4}, \quad i \in [D_1] \end{aligned}$$

for  $x \in [\underline{T}_i, \bar{T}_i]$ . Combining (23) with the last display, we have

$$|e^{-x} - e^{-\underline{T}_i} f_i(x)| \leq |e^{-x} - e^{-\underline{T}_i} P_i(x)| + |P_i(x) - f_i(x)| \leq \frac{\epsilon}{4} + \frac{\epsilon^2}{4} \leq \frac{\epsilon}{2}, \quad i \in [D_1] \quad (26)$$

for  $x \in [\underline{T}_i, \bar{T}_i]$ , where the first inequality holds because  $e^{-\underline{T}_i} \leq 1$ . Consider functions  $f_{\text{swit}}^{(1)}, \dots, f_{\text{swit}}^{(D_1+1)} : \mathbb{R} \rightarrow [0, 1]$  such that

$$\begin{aligned} f_{\text{swit}}^{(1)}(\cdot) &= \frac{1}{\bar{T}_1 - \underline{T}_2} \rho\left(-f_{\text{clip}}^{(\underline{T}_2, \bar{T}_1)}(\cdot) + \bar{T}_1\right), \\ f_{\text{swit}}^{(i)}(\cdot) &= \frac{1}{\bar{T}_{i-1} - \underline{T}_i} \rho\left(f_{\text{clip}}^{(\underline{T}_i, \bar{T}_{i-1})}(\cdot) - \underline{T}_i\right) - \frac{1}{\bar{T}_i - \underline{T}_{i+1}} \rho\left(f_{\text{clip}}^{(\underline{T}_{i+1}, \bar{T}_i)}(\cdot) - \underline{T}_{i+1}\right), \\ 2 \leq i \leq D_1, \\ f_{\text{swit}}^{(D_1+1)}(\cdot) &= \frac{1}{\bar{T}_{D_1} - \underline{T}_{D_1+1}} \rho\left(f_{\text{clip}}^{(\underline{T}_{D_1+1}, \bar{T}_{D_1})}(\cdot) - \underline{T}_{D_1+1}\right), \end{aligned}$$

where  $\underline{T}_{D_1+1} = D_1$  and  $f_{\text{clip}}^{(\underline{T}_i, \bar{T}_{i-1})} \in \mathcal{F}_{\text{NN}}(2, (1, 2, 1)^\top, 7, D_1)$  denotes the neural network in Lemma 15. Note that  $\sum_{i=1}^{D_1+1} f_{\text{swit}}^{(i)}(x) = 1$  for  $x \in \mathbb{R}$ , and  $f_{\text{swit}}^{(i)}(x) = 0$  for  $x \in [0, \underline{T}_i] \cup [\bar{T}_i, \infty)$ ,  $i \in [D_1]$  and  $f_{\text{swit}}^{(D_1+1)}(x) = 0$  for  $x \leq \underline{T}_{D_1+1}$ . Consider a function  $f : \mathbb{R} \rightarrow \mathbb{R}$  such that  $f(\cdot) = \sum_{i=1}^{D_1} e^{-\underline{T}_i} f_{\text{mult}}^{(2)}(f_{\text{swit}}^{(i)}(\cdot), f_i(\cdot))$ . Since  $|f_{\text{mult}}^{(2)}(x_1, x_2) - x_1 x_2| \leq \epsilon^2/(4D_2)$  for any  $x_1, x_2 \in [-2, 2]$ , we have

$$\begin{aligned} |e^{-x} - f(x)| &\leq \left| e^{-x} - \sum_{i=1}^{D_1} e^{-\underline{T}_i} f_{\text{swit}}^{(i)}(x) f_i(x) \right| + \frac{D_1 \epsilon^2}{4D_2} \\ &= \left| \sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) \{e^{-x} - e^{-\underline{T}_i} f_i(x)\} + f_{\text{swit}}^{(D_1+1)}(x) e^{-x} \right| + \frac{D_1 \epsilon^2}{4D_2}, \\ &\leq \sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) |e^{-x} - e^{-\underline{T}_i} f_i(x)| + \frac{\epsilon}{4} + \frac{D_1 \epsilon^2}{4D_2} \\ &\leq \frac{\epsilon}{2} \sum_{i=1}^{D_1} f_{\text{swit}}^{(i)}(x) + \frac{\epsilon}{4} + \frac{D_1 \epsilon^2}{4D_2} \leq \left( \frac{3}{4} + \frac{(D_1 + 1)\epsilon}{4D_2} \right) \epsilon \leq \epsilon \end{aligned}$$

for  $x \in [0, \infty)$ , where the second inequality holds because  $|f_{\text{swit}}^{(D_1+1)}(x) e^{-x}| \leq e^{-x} \leq \epsilon/4$  for  $x \geq \underline{T}_{D_1+1}$  and the third inequality holds by (26). Combining (24) and (25) with Lemma 10 and Lemma 9, we have  $f_{\text{mult}}^{(2)}(f_{\text{swit}}^{(i)}(\cdot), f_i(\cdot)) \in \mathcal{F}_{\text{NN}}(\tilde{L}^{(i)}, \tilde{\mathbf{d}}^{(i)}, \tilde{s}^{(i)}, \tilde{M}^{(i)})$  for  $i \in [D_1]$  with

$$\begin{aligned} \tilde{L}^{(i)} &\leq (L^{(i)} \vee 2) + L_{\text{mult}}^{(2)} \leq D_4 \log D_2 \{\log(1/\epsilon) + \log D_2\} \\ \|\tilde{\mathbf{d}}^{(i)}\|_\infty &\leq 2 \max\left(2\|\mathbf{d}^{(i)}\|_\infty + 4, \|\mathbf{d}_{\text{mult}}^{(2)}\|_\infty\right) \leq D_4 D_2^2 \\ \tilde{s}^{(i)} &\leq 4s^{(i)} + 4(L^{(i)} \vee 2) + 2s_{\text{mult}}^{(2)} + 28 \leq D_4 D_2^2 \{\log(1/\epsilon) + D_2\} \\ \tilde{M}^{(i)} &\leq \max\left(D_1, M^{(i)}, M_{\text{mult}}^{(2)}, 1\right), \end{aligned}$$

where  $D_4 = D_4(D_3)$  is a large enough constant. Since  $f$  is a linear combination of  $f_{\text{mult}}^{(2)}(f_{\text{swit}}^{(i)}(\cdot), f_i(\cdot))$  for each  $i \in [D_1]$ , Lemma 9, Lemma 10 and Lemma 11 implies that  $f \circ \rho_1 \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with

$$\begin{aligned} L &\leq \max_{i \in [D_1]} \tilde{L}^{(i)} + 3 \leq D_5 \log(1/\epsilon) \log \log(1/\epsilon) \\ \|\mathbf{d}\|_\infty &\leq 2 \max \left( 2 \sum_{i=1}^{D_1} \|\tilde{\mathbf{d}}^{(i)}\|_\infty, 4D_1 \right) \leq D_5 \{\log(1/\epsilon)\}^3 \\ s &\leq 2 \sum_{i=1}^{D_1} \left( \tilde{s}^{(i)} + \max_{j \in [D_1]} \tilde{L}^{(j)} \right) + 4D_1 + 4 \leq D_5 \{\log(1/\epsilon)\}^4 \\ M &\leq \max_{i \in [D_1]} \left( \tilde{M}^{(i)} \vee e^{-T_i} \right) \leq D_5 \epsilon^{-1} \end{aligned}$$

for large enough constant  $D_5 = D_5(D_4)$ . Note that  $|(f \circ \rho_1)(\tilde{x}) - e^{-x}| \leq |(f \circ \rho_1)(\tilde{x}) - e^{-(\tilde{x} \vee 0)}| + |e^{-(\tilde{x} \vee 0)} - e^{-x}| \leq \epsilon + |x - \tilde{x}|$  for any  $x \geq 0$  and  $\tilde{x} \in \mathbb{R}$ . Then, the assertion follows by re-defining the constant.  $\blacksquare$

**Lemma 18** ( $\mu_t$  and  $\sigma_t$ ) *For any  $0 < \epsilon < 1/2$ , there exists a positive constant  $C_{N,4} = C_{N,4}(\underline{\tau}, \bar{\tau})$  and neural networks  $f_\mu \in \mathcal{F}_{\text{NN}}(L_\mu, \mathbf{d}_\mu, s_\mu, M_\mu)$ ,  $f_\sigma \in \mathcal{F}_{\text{NN}}(L_\sigma, \mathbf{d}_\sigma, s_\sigma, M_\sigma)$  with*

$$\begin{aligned} L_\mu, L_\sigma &\leq C_{N,4} \{\log(1/\epsilon)\}^2, \quad \|\mathbf{d}_\mu\|_\infty, \|\mathbf{d}_\sigma\|_\infty \leq C_{N,4} \{\log(1/\epsilon)\}^2 \\ s_\mu, s_\sigma &\leq C_{N,4} \{\log(1/\epsilon)\}^3, \quad M_\mu, M_\sigma \leq C_{N,4} \log(1/\epsilon) \end{aligned}$$

such that

$$|\mu_{t_1} - f_\mu(t_1)| \leq \epsilon \quad \text{and} \quad |\sigma_{t_2} - f_\sigma(t_2)| \leq \epsilon$$

for any  $t_1 \geq 0$  and  $t_2 \geq \epsilon$ .

**Proof** This is a re-statement of Lemma B.1 in Oko et al. (2023).  $\blacksquare$

**Lemma 19 (Reciprocal function)** *For any  $0 < \epsilon < 1$ , there exists a positive constant  $C_{N,5}$  and a neural network  $f_{\text{rec}} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with*

$$\begin{aligned} L &\leq C_{N,5} \{\log(1/\epsilon)\}^2, \quad \|\mathbf{d}\|_\infty \leq C_{N,5} \{\log(1/\epsilon)\}^3 \\ s &\leq C_{N,5} \{\log(1/\epsilon)\}^4, \quad M \leq C_{N,5} \epsilon^{-2} \end{aligned}$$

such that

$$\left| \frac{1}{x} - f_{\text{rec}}(\tilde{x}) \right| \leq \epsilon + \frac{|x - \tilde{x}|}{\epsilon^2}$$

for any  $x \in [\epsilon, 1/\epsilon]$  and  $\tilde{x} \in \mathbb{R}$ .

**Proof** This is a re-statement of Lemma F.7 in Oko et al. (2023).  $\blacksquare$

## Appendix B. Proofs for the Approximation Theory

In this section, we provide the proof of Theorem 5. We begin by outlining the crucial lemmas and propositions.

For  $n \in \mathbb{N}$ , let  $P_n$  be the Legendre polynomial of degree  $n$  defined as

$$P_n(x) = \left( \frac{1}{2^n n!} \right) \frac{d^n}{dx^n} (x^2 - 1)^n$$

for  $x \in \mathbb{R}$ . It is well-known (page 114 of Arnold (2004)) that equation  $P_n = 0$  has  $n$  distinct roots  $\tilde{x}_1^{(n)}, \dots, \tilde{x}_n^{(n)}$  satisfying  $-1 < \tilde{x}_1^{(n)} < \dots < \tilde{x}_n^{(n)} < 1$ . Let  $\{\tilde{w}_1^{(n)}, \dots, \tilde{w}_n^{(n)}\}$  be the Gauss-Legendre quadrature weights, that is,

$$\tilde{w}_j^{(n)} = \begin{cases} \int_{-1}^1 \prod_{\substack{k=1 \\ k \neq j}}^n \left( \frac{x - \tilde{x}_k^{(n)}}{\tilde{x}_j^{(n)} - \tilde{x}_k^{(n)}} \right) dx, & \text{if } n \geq 2 \\ 2, & \text{if } n = 1. \end{cases}$$

Let  $n_\beta$  be the largest integer strictly smaller than  $\beta \vee 2$ . For simplicity, we denote the vectors  $(\tilde{x}_1^{(n_\beta)}, \dots, \tilde{x}_{n_\beta}^{(n_\beta)})$  and  $(\tilde{w}_1^{(n_\beta)}, \dots, \tilde{w}_{n_\beta}^{(n_\beta)})$  as  $(\tilde{x}_1, \dots, \tilde{x}_{n_\beta})$  and  $(\tilde{w}_1, \dots, \tilde{w}_{n_\beta})$ , respectively. The following lemma provides an error bound for the  $m$ -points quadrature rule to approximate a one-dimensional integral.

**Lemma 20 (1-dimensional  $m$ -point quadrature rule)** *Let  $A < B$  and  $\beta, K > 0$  be given. For every  $m \in n_\beta \mathbb{N}$ , there exists  $(w_i, x_i)_{i \in [m]}$  with  $w_i > 0$  and  $x_i \in (A, B)$  such that*

$$\left| \int_A^B g(x) dx - \sum_{i=1}^m w_i g(x_i) \right| \leq \left\{ \frac{n_\beta^\beta}{2^{\beta - \lfloor \beta \rfloor} \lfloor \beta \rfloor!} \right\} K (B - A)^{\beta+1} m^{-\beta},$$

for every  $g \in \mathcal{H}_1^{\beta, K}([A, B])$ . More specifically, one can choose

$$w_i = \frac{(B - A) n_\beta}{2m} \tilde{w}_{i - n_\beta \lfloor i/n_\beta \rfloor},$$

$$x_i = A + \frac{(B - A) n_\beta}{2m} \left\{ \tilde{x}_{i - n_\beta \lfloor i/n_\beta \rfloor} + 2 \lfloor i/n_\beta \rfloor + 1 \right\}.$$

Let  $\phi$  be the one-dimensional standard normal density. The following lemma provides a bound for the Hölder-norm of a function multiplied by  $\phi$  and its derivative  $\phi'$ .

**Lemma 21 (Preservation of Hölder continuity)** *Let  $\beta, K > 0, a, b \in \mathbb{R}$  be given and  $g \in \mathcal{H}_1^{\beta, K}([a, b])$ . Then, there exists a positive constant  $C_{G,1} = C_{G,1}(\beta)$  such that  $g\phi \in \mathcal{H}_1^{\beta, K C_{G,1}}([a, b])$  and  $g\phi' \in \mathcal{H}_1^{\beta, K C_{G,1}}([a, b])$ .*

For  $\mu, \sigma > 0$ , define  $p_{\mu, \sigma}(\cdot)$  as

$$p_{\mu, \sigma}(\mathbf{x}) = \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \phi_\sigma(\mathbf{x} - \mu \mathbf{y}) d\mathbf{y} = \mu^{-D} \int_{\|\mathbf{x} + \sigma \mathbf{y}\|_\infty \leq \mu} p_0 \left( \frac{\mathbf{x} + \sigma \mathbf{y}}{\mu} \right) \prod_{i=1}^D \phi(y_i) d\mathbf{y}.$$

Since  $p_0$  is  $\beta$ -smooth under the **(S)** assumption, we can approximate the integral using the quadrature method with Lemma 20 and Lemma 21. Note however that  $\mathbf{y}$  in RHS ranges over a large set for small  $\sigma$ , and the error bound given in Lemma 20 depends polynomially on the size of the interval. Since the tail of  $\phi$  decays very quickly, one can control the numerical error as in the following lemma.

**Lemma 22 (Quadrature rule for  $p_{\mu,\sigma}(\mathbf{x})$  and  $\nabla p_{\mu,\sigma}(\mathbf{x})$ )** *Let  $\beta, K > 0$  be given and suppose that true density  $p_0$  belongs to  $\mathcal{H}^{\beta,K}([-1,1]^D)$ . For  $\tau_{\text{bd}}, \tau_{\text{tail}}, \mu, \sigma > 0$ ,  $m \in n_\beta \mathbb{N}$ ,  $i \in [D]$ ,  $j \in [m]$  and  $\mathbf{x} = (x_1, \dots, x_D)^\top \in \mathbb{R}^D$ , let*

$$y_j^{(i)} = 2\sqrt{2\tau_{\text{tail}}}\{\log(1/\sigma)\}^{\tau_{\text{bd}}+\frac{1}{2}} \left\{ -x_i - \mu + \frac{n_\beta \mu}{m} \left( \tilde{x}_{j-n_\beta \lfloor j/n_\beta \rfloor} + 2 \lfloor j/n_\beta \rfloor + 1 \right) \right\},$$

$$w_j = 2\sqrt{2\tau_{\text{tail}}} n_\beta \tilde{w}_{j-n_\beta \lfloor j/n_\beta \rfloor} \{\log(1/\sigma)\}^{\tau_{\text{bd}}+\frac{1}{2}}.$$

For  $\mathbf{j} = (j_1, \dots, j_D)^\top \in [m]^D$ , let  $\tilde{\mathbf{y}}_{\mathbf{j}} = (y_{j_1}^{(1)}, \dots, y_{j_D}^{(D)})^\top \in \mathbb{R}^D$ . Then,

$$\left\| \frac{\mathbf{x} + \sigma \tilde{\mathbf{y}}_{\mathbf{j}}}{\mu} \right\|_\infty \leq 1 - \frac{\{\log(1/\sigma)\}^{-\tau_{\text{bd}}}}{2}, \quad \mathbf{j} \in [m]^D,$$

$$\mu^D \left| p_{\mu,\sigma}(\mathbf{x}) - \frac{1}{m^D} \sum_{\mathbf{j} \in [m]^D} \left\{ \prod_{i=1}^D w_{j_i} \phi(y_{j_i}^{(i)}) \right\} p_0 \left( \frac{\mathbf{x} + \sigma \tilde{\mathbf{y}}_{\mathbf{j}}}{\mu} \right) \right| \leq \epsilon \quad \text{and}$$

$$\mu^D \left\| \sigma \nabla p_{\mu,\sigma}(\mathbf{x}) - \frac{1}{m^D} \sum_{\mathbf{j} \in [m]^D} \tilde{\mathbf{y}}_{\mathbf{j}} \left\{ \prod_{i=1}^D w_{j_i} \phi(y_{j_i}^{(i)}) \right\} p_0 \left( \frac{\mathbf{x} + \sigma \tilde{\mathbf{y}}_{\mathbf{j}}}{\mu} \right) \right\|_\infty \leq \epsilon$$

for every  $\|\mathbf{x}\|_\infty \leq \mu - \mu \{\log(1/\sigma)\}^{-\tau_{\text{bd}}}$ ,  $\mu \in [1/2, 1]$ ,  $\sigma \in (0, \tilde{C}_2]$ , where  $\tilde{C}_1 = \tilde{C}_1(\beta, D, \tau_{\text{tail}})$ ,  $\tilde{C}_2 = \tilde{C}_2(\beta, D, \tau_{\text{bd}}, \tau_{\text{tail}})$  and

$$\epsilon = \tilde{C}_1 K \left( \sigma^{\tau_{\text{tail}}} + m^{-\beta} \{\log(1/\sigma)\}^{(\tau_{\text{bd}}+\frac{1}{2})(\beta+1)} \right) \{\log(1/\sigma)\}^{(\tau_{\text{bd}}+\frac{1}{2})(D-1)}.$$

We can approximate the maps  $(\mathbf{x}, t) \mapsto p_t(\mathbf{x})$  and  $(\mathbf{x}, t) \mapsto \nabla p_t(\mathbf{x})$  using deep ReLU networks by replacing  $(\mu, \sigma)$  in Lemma 22 with  $(\mu_t, \sigma_t)$ . As discussed in Section 5.3, a weight-sharing network is used to reduce the number of distinct network parameters. The approximation result is provided in the following proposition.

**Proposition 23 (Approximation at the interior of near-support)** *Suppose the true density  $p_0$  satisfies the assumption **(S)** and*

$$\tau_{\text{bd}} \in 1/2 + \mathbb{N}, \quad \tau_{\text{tail}} > 0, \quad \tau_{\text{min}} \geq \frac{4\beta}{d(\beta \wedge 1)}.$$

Then, for every  $m \geq \tilde{C}_5$ , there exists a class of permutation matrices  $\mathcal{P} = \{\mathcal{Q}_i, \mathcal{R}_i\}_{i \in [L-1]}$  and weight-sharing network  $\mathbf{f} \in \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  with

$$L \leq \tilde{C}_3 (\log m)^2 \log \log m, \quad \|\mathbf{d}\|_\infty \leq \tilde{C}_3 m^{D+1},$$

$$s \leq \tilde{C}_3 m (\log m)^5 \log \log m, \quad M \leq \exp \left( \tilde{C}_3 \{\log m\}^2 \right),$$

$$\|\mathbf{m}\|_\infty \leq \tilde{C}_3 m^D$$

satisfying

$$\left\| \begin{pmatrix} \sigma_t \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} - \mathbf{f}(\mathbf{x}, t) \right\|_{\infty} \leq \tilde{C}_4 (\log m)^{(\tau_{\text{bd}} + \frac{1}{2})(D-1)} \left\{ t^{\frac{\tau_{\text{tail}}}{2}} + m^{-\frac{\beta}{d}} (\log m)^{(\tau_{\text{bd}} + \frac{1}{2})(\beta+1)} \right\}$$

for every  $\mathbf{x} \in \mathbb{R}^D$  with  $\|\mathbf{x}\|_{\infty} \leq \mu_t - \mu_t \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $m^{-\tau_{\text{min}}} \leq t \leq \bar{\tau}^{-1}(\tilde{C}_2^2 \wedge 1/2)$ .

Here,  $\tilde{C}_3 = \tilde{C}_3(\beta, d, D, K, \bar{\tau}, \underline{\tau}, \tau_{\text{bd}}, \tau_{\text{tail}}, \tau_{\text{min}})$ ,  $\tilde{C}_4 = \tilde{C}_4(\beta, d, D, K, \underline{\tau}, \tau_{\text{bd}}, \tau_{\text{tail}}, \tau_{\text{min}})$ ,  $\tilde{C}_5 = \tilde{C}_5(\beta, d, \underline{\tau}, \tau_{\text{bd}}, \tau_{\text{tail}}, \tau_{\text{min}})$  and  $\tilde{C}_2 = \tilde{C}_2(\beta, D, \tau_{\text{bd}}, \tau_{\text{tail}})$  be the constant in Lemma 22,

As  $t \rightarrow 0$ ,  $p_t$  is not lower bounded near the boundary of the support of  $p_0$  due to the lower bound condition, making the approximation of  $\nabla \log p_t$  challenging. With the assumption **(B)**,  $p_0$  is infinitely smooth so one can approximate  $p_0$  efficiently with local polynomials by applying Taylor's theorem in the low-density region. Since a Gaussian density can also be efficiently approximated with local polynomials, one can calculate the integral in  $p_t$  closed form, and approximate the output with vanilla feedforward neural networks. The following proposition provides the approximation result, and our main proof strategy follows the proofs of Lemma B.2–Lemma B.5 from Oko et al. (2023), with modifications for simplification.

**Proposition 24 (Approximation at the boundary of near-support)** *Let  $K, \tau_{\text{bd}}, \tau_x > 0$ ,  $0 < \tau_t < 1$ ,  $0 < \tilde{\tau}_{\text{bd}} < \tau_{\text{bd}}$  be given and suppose the true density  $p_0$  satisfies that  $\|p_0\|_{\infty} \leq K$ . Then, for  $0 < \delta \leq \tilde{C}_8$  and  $p_0$  satisfying*

$$\sup_{\alpha \in \mathbb{N}^D} \sup_{1 - \{\log(1/\delta)\}^{-\tilde{\tau}_{\text{bd}}} \leq \|\mathbf{x}\|_{\infty} \leq 1} |(D^{\alpha} p_0)(\mathbf{x})| \leq K,$$

there exists a network  $\mathbf{f} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with

$$\begin{aligned} L &\leq \tilde{C}_6 \{\log(1/\delta)\}^4, \quad \|\mathbf{d}\|_{\infty} \leq \tilde{C}_6 \{\log(1/\delta)\}^{7+D\tilde{\tau}_{\text{bd}}+D}, \\ s &\leq \tilde{C}_6 \{\log(1/\delta)\}^{11+D\tilde{\tau}_{\text{bd}}+D}, \quad M \leq \exp\left(\tilde{C}_6 \{\log(1/\delta)\}^2\right), \end{aligned}$$

satisfying

$$\left\| \begin{pmatrix} \sigma_t \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} - \mathbf{f}(\mathbf{x}, t) \right\|_{\infty} \leq \tilde{C}_7 \delta \{\log(1/\delta)\}^D$$

for every  $\mathbf{x} \in \mathbb{R}^D$  with  $\mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}} \leq \|\mathbf{x}\|_{\infty} \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \delta^{\tau_t}$ .

Here,  $\tilde{C}_6 = \tilde{C}_6(D, K, \bar{\tau}, \underline{\tau}, \tau_x)$ ,  $\tilde{C}_7 = \tilde{C}_7(D, K, \underline{\tau})$ ,  $\tilde{C}_8 = \tilde{C}_8(D, \bar{\tau}, \tau_{\text{bd}}, \tau_x, \tau_t, \tilde{\tau}_{\text{bd}})$  are positive constants.

For  $t_* \geq 0$  and  $t > 0$ , we have

$$p_{t_*+t}(\mathbf{x}) = \int_{\mathbb{R}^D} p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y}, \quad \mathbf{x} \in \mathbb{R}^D$$

due to the Markov property of the process  $(\mathbf{X}_t)_{t \geq 0}$ . Note that the map  $\mathbf{x} \mapsto p_{t_*}(\mathbf{x})$  is infinitely differentiable and its norm is bounded as  $\|D^{\mathbf{k}} p_{t_*}(\cdot)\|_{\infty} \lesssim t_*^{-k/2}$  for any  $\mathbf{k} \in \mathbb{N}^D$ ; see

Lemma 8). Then, one can approximate  $p_{t_*}$  with a local Taylor expansion, yielding an error  $O(m^{-k./D}t_*^{-k./2})$  using grid points bounded by  $O(m)$ , both up to a poly-logarithmic factor. Similar to the proof of Proposition 24, one can approximate the map  $(\mathbf{x}, t) \mapsto p_{t_*+t}(\mathbf{x})$  with vanilla feedforward neural networks. The following proposition provides the approximation result, and our main proof strategy follows the proof of Lemma B.7 from Oko et al. (2023), with modifications for simplification.

**Proposition 25 (Approximation for large  $t$ )** *Let  $K, \tau_1, \tau_x > 0, \tau_{\text{sm}} \in \mathbb{N}, \tau_{\text{low}} \in (0, 1)$  be given and suppose the true density  $p_0$  satisfies that  $\tau_1 \leq p_0(\mathbf{x}) \leq K$  for any  $\mathbf{x} \in [-1, 1]^D$ . Then, for  $m \geq \tilde{C}_{11}$ , there exists a neural network  $\mathbf{f} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with*

$$\begin{aligned} L &\leq \tilde{C}_9(\log m)^4, & \|\mathbf{d}\|_\infty &\leq \tilde{C}_9 m(\log m)^9, \\ s &\leq \tilde{C}_9 m(\log m)^9, & M &\leq \exp(\tilde{C}_9(\log m)^2) \end{aligned}$$

such that

$$\left\| \begin{pmatrix} \sigma_t \nabla p_{t_*+t}(\mathbf{x}) \\ p_{t_*+t}(\mathbf{x}) \end{pmatrix} - \mathbf{f}(\mathbf{x}, t) \right\|_\infty \leq \tilde{C}_{10} m^{-\frac{\tau_{\text{low}} \tau_{\text{sm}} - (D+1-\tau_{\text{low}})D}{D(1+D)}} (\log m)^{D(\frac{\tau_{\text{sm}}}{2}+1)}$$

for every  $\mathbf{x} \in \mathbb{R}^D$  with  $\|\mathbf{x}\|_\infty \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$ ,  $\delta \leq t \leq \bar{\tau}^{-1} \log(1/\delta)$ , where

$$t_* = m^{-\frac{2-2\tau_{\text{low}}}{D}} \quad \text{and} \quad \delta = m^{-\frac{\tau_{\text{low}} \tau_{\text{sm}} + D + 1 - \tau_{\text{low}}}{D(1+D)}}.$$

Here,  $\tilde{C}_9, \tilde{C}_{10}, \tilde{C}_{11}$  are positive constants depending on  $(D, K, \bar{\tau}, \underline{\tau}, \tau_x, \tau_{\text{sm}}, \tau_{\text{low}})$ .

## B.1 Proofs of Lemma 20 to 22

In this subsection, we provide the proof of Lemma 20, Lemma 21, and Lemma 22.

By the definition, we have  $\exp(-\bar{\tau}t) \leq \mu_t \leq \exp(-\underline{\tau}t)$  and  $1 - \exp(-2\bar{\tau}t) \leq \sigma_t^2 \leq 1 - \exp(-2\underline{\tau}t)$  for  $t \geq 0$ . Since  $x/2 \leq 1 - e^{-x}$  for  $0 \leq x \leq 1$  and  $1 - e^{-x} \leq x$  for  $x \geq 0$ , we have

$$\begin{aligned} \mu_t &\leq 1 - \frac{\tau t}{2} \leq 1, & \sigma_t &\leq \sqrt{1 - \exp(-2\bar{\tau}t)} \leq \sqrt{2\bar{\tau}t}, & \forall t \geq 0, & \text{ and} \\ \mu_t &\geq 1 - \bar{\tau}t \geq \frac{1}{2}, & \sigma_t &\geq \sqrt{1 - \exp(-2\underline{\tau}t)} \geq \sqrt{\underline{\tau}t}, & \forall 0 \leq t \leq (2\bar{\tau})^{-1}. \end{aligned} \tag{27}$$

The last display is widely used in the following proofs.

### B.1.1 PROOF OF LEMMA 20

**Proof** Let  $m_0 = \frac{2m}{(B-A)n_\beta}$  and consider a function  $g \in \mathcal{H}_1^{\beta, K}([A, B])$ . Simple calculation yields that

$$\int_A^B g(x) dx = \sum_{i=1}^{\frac{m_0(B-A)}{2}} \int_{A+\frac{2(i-1)}{m_0}}^{A+\frac{2i}{m_0}} g(x) dx = \sum_{i=1}^{\frac{m_0(B-A)}{2}} \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} g_i(x) dx, \tag{28}$$

where  $g_i(x) = g(x + A + \frac{2i-1}{m_0})$ . For each  $i \in \{1, \dots, \frac{m_0(B-A)}{2}\}$ , let  $L_i$  be the Lagrange interpolating polynomial of degree  $n_\beta - 1$  that agrees with the function  $g_i$  at knots  $\{\tilde{x}_1/m_0, \dots, \tilde{x}_{n_\beta}/m_0\}$ , defined as

$$L_i(x) = \sum_{j=1}^{n_\beta} g_i(\tilde{x}_j/m_0) l_j(x),$$

where

$$l_j(x) = \begin{cases} \prod_{\substack{k=1 \\ k \neq j}}^{[\beta]} \frac{m_0 x - \tilde{x}_k}{\tilde{x}_j - \tilde{x}_k}, & \text{if } \beta > 2, \\ 1, & \text{if } 0 < \beta \leq 2, \end{cases}$$

for  $j \in [n_\beta]$ . Note that  $L_i(\tilde{x}_j/m_0) = g_i(\tilde{x}_j/m_0)$  for any  $j \in [n_\beta]$ .

If  $0 < \beta \leq 1$ ,  $\tilde{x}_1 = 0$  and  $L_i(x) = g_i(0)$ . Since  $g_i \in \mathcal{H}_1^{\beta, K}([-1/m_0, 1/m_0])$ , we have

$$\begin{aligned} \left| \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} \{g_i(x) - L_i(x)\} dx \right| &\leq \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} |g_i(x) - L_i(x)| dx \\ &\leq \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} K|x|^\beta dx \leq \frac{2}{m_0} K m_0^{-\beta} = 2K m_0^{-(\beta+1)}. \end{aligned} \quad (29)$$

If  $\beta > 1$ , fix  $\tilde{x}_0 \in [-1, 1]$  satisfying  $\tilde{x}_0 \neq \tilde{x}_j$  for  $j \in [[\beta]]$ . Consider a function  $h : [-1/m_0, 1/m_0] \rightarrow \mathbb{R}$  such that

$$h(x) = g_i(x) - L_i(x) - \left\{ g_i\left(\frac{\tilde{x}_0}{m_0}\right) - L_i\left(\frac{\tilde{x}_0}{m_0}\right) \right\} \prod_{j=1}^{[\beta]} \left( \frac{m_0 x - \tilde{x}_j}{\tilde{x}_0 - \tilde{x}_j} \right).$$

Then,  $h(\tilde{x}_j/m_0) = 0$  for  $j \in \{0, \dots, [\beta]\}$  and  $g$  is  $[\beta]$ -times differentiable on  $(-1/m_0, 1/m_0)$ . Generalized Rolle's Theorem (see Theorem 1.10 of Burden and Faires (2010)) implies that there exists a constant  $\xi_{\tilde{x}_0} \in (-1/m_0, 1/m_0)$  such that  $(D^{[\beta]}h)(\xi_{\tilde{x}_0}) = 0$ . Since  $L_i$  is the polynomial of degree less than  $[\beta]$  and  $(D^{[\beta]}L_i)(\xi_{\tilde{x}_0}) = 0$ , a simple calculation yields that

$$g_i\left(\frac{\tilde{x}_0}{m_0}\right) = L_i\left(\frac{\tilde{x}_0}{m_0}\right) + \frac{(D^{[\beta]}g_i)(\xi_{\tilde{x}_0})}{[\beta]!} \prod_{j=1}^{[\beta]} \left( \frac{\tilde{x}_0 - \tilde{x}_j}{m_0} \right).$$

Note that  $g_i(\tilde{x}_j/m_0) = L_i(\tilde{x}_j/m_0)$  for  $j \in [[\beta]]$ . Combining with the last display, there exists a function  $\xi : [-1/m_0, 1/m_0] \rightarrow (-1/m_0, 1/m_0)$  such that

$$g_i(x) = L_i(x) + \frac{(D^{[\beta]}g_i)(\xi(x))}{[\beta]!} \prod_{j=1}^{[\beta]} \left( x - \frac{\tilde{x}_j}{m_0} \right), \quad x \in \left[ -\frac{1}{m_0}, \frac{1}{m_0} \right],$$

where  $\xi(x) = 0$  for  $x \in \{\frac{\tilde{x}_1}{m_0}, \dots, \frac{\tilde{x}_{\lfloor \beta \rfloor}}{m_0}\}$ . For  $x \in [-1/m_0, 1/m_0]$ , we have

$$\begin{aligned} & \left| g_i(x) - L_i(x) - \frac{(D^{\lfloor \beta \rfloor} g_i)(0)}{\lfloor \beta \rfloor!} \prod_{j=1}^{\lfloor \beta \rfloor} \left( x - \frac{\tilde{x}_j}{m_0} \right) \right| \\ &= \left| \left\{ \frac{(D^{\lfloor \beta \rfloor} g_i)(\xi(x)) - (D^{\lfloor \beta \rfloor} g_i)(0)}{\lfloor \beta \rfloor!} \right\} \prod_{j=1}^{\lfloor \beta \rfloor} \left( x - \frac{\tilde{x}_j}{m_0} \right) \right| \\ &\leq \frac{K|\xi(x)|^{\beta - \lfloor \beta \rfloor}}{\lfloor \beta \rfloor!} \prod_{j=1}^{\lfloor \beta \rfloor} \left( \frac{2}{m_0} \right) \leq \frac{K2^{\lfloor \beta \rfloor}}{\lfloor \beta \rfloor!} m_0^{-\beta}, \end{aligned}$$

where the first inequality holds because  $g_i \in \mathcal{H}_1^{\beta, K}([-1/m_0, 1/m_0])$ . Since  $\{\tilde{x}_1, \dots, \tilde{x}_{\lfloor \beta \rfloor}\}$  are the roots of the Legendre polynomial, its orthogonality implies that  $\int_{-1/m_0}^{1/m_0} \prod_{j=1}^{\lfloor \beta \rfloor} (x - \frac{\tilde{x}_j}{m_0}) dx = 0$ . Combining with the last display, it follows that

$$\begin{aligned} & \left| \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} \{g_i(x) - L_i(x)\} dx \right| \\ &= \left| \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} \left\{ g_i(x) - L_i(x) - \frac{(D^{\lfloor \beta \rfloor} g_i)(0)}{\lfloor \beta \rfloor!} \prod_{j=1}^{\lfloor \beta \rfloor} \left( x - \frac{\tilde{x}_j}{m_0} \right) \right\} dx \right| \tag{30} \\ &\leq \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} \left| g_i(x) - L_i(x) - \frac{(D^{\lfloor \beta \rfloor} g_i)(0)}{\lfloor \beta \rfloor!} \prod_{j=1}^{\lfloor \beta \rfloor} \left( x - \frac{\tilde{x}_j}{m_0} \right) \right| dx \leq \frac{K2^{\lfloor \beta \rfloor + 1}}{\lfloor \beta \rfloor!} m_0^{-(\beta + 1)}. \end{aligned}$$

A simple calculation yields that

$$\int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} L_i(x) dx = \sum_{j=1}^{n_\beta} g_i \left( \frac{\tilde{x}_j}{m_0} \right) \left\{ \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} l_j(x) dx \right\} = \sum_{j=1}^{n_\beta} \frac{\tilde{w}_j}{m_0} g_i \left( \frac{\tilde{x}_j}{m_0} \right).$$

Combining (28), (29) and (30) with the last display, we have

$$\begin{aligned} & \left| \int_A^B g(x) dx - \sum_{i=1}^{\frac{m_0(B-A)}{2}} \sum_{j=1}^{n_\beta} \frac{\tilde{w}_j}{m_0} g_i \left( \frac{\tilde{x}_j}{m_0} \right) \right| \leq \sum_{i=1}^{\frac{m_0(B-A)}{2}} \left| \int_{-\frac{1}{m_0}}^{\frac{1}{m_0}} \{g_i(x) - L_i(x)\} dx \right| \\ &\leq \frac{K(B-A)2^{\lfloor \beta \rfloor}}{\lfloor \beta \rfloor!} m_0^{-\beta} = \frac{(\lfloor \beta \rfloor \vee 1)^\beta}{2^{\beta - \lfloor \beta \rfloor} \lfloor \beta \rfloor!} (B-A)^{\beta + 1} m_0^{-\beta}. \end{aligned}$$

Then, the assertion follows because  $\sum_{i=1}^m w_i g(x_i) = \sum_{i=1}^{m_0(B-A)/2} \sum_{j=1}^{n_\beta} \frac{\tilde{w}_j}{m_0} g_i \left( \frac{\tilde{x}_j}{m_0} \right)$ . ■

## B.1.2 PROOF OF LEMMA 21

**Proof** For any  $n \in \mathbb{Z}_{\geq 0}$ , it is well-known (see (Indritz, 1961)) that

$$\left| \frac{d^n}{dx^n} e^{-x^2} \right| \leq \sqrt{2^n n!} e^{-\frac{x^2}{2}}, \quad x \in \mathbb{R}$$

and moreover,

$$\|D^n \phi\|_\infty = \frac{1}{\sqrt{2\pi}} \left\| \frac{d^n}{dx^n} e^{-\frac{x^2}{2}} \right\|_\infty \leq \frac{\sqrt{n!}}{\sqrt{2\pi}} \left\| e^{-\frac{x^2}{4}} \right\|_\infty \leq \frac{\sqrt{n!}}{\sqrt{2\pi}}, \quad (31)$$

where the first inequality holds by the chain rule. Then,

$$\begin{aligned} \sum_{\alpha=0}^{\lfloor \beta \rfloor} \|D^\alpha(g\phi)\|_\infty &= \sum_{\alpha=0}^{\lfloor \beta \rfloor} \left\| \sum_{r=0}^{\alpha} \binom{\alpha}{r} (D^r g)(D^{\alpha-r} \phi) \right\|_\infty \\ &\leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} \sum_{r=0}^{\alpha} \binom{\alpha}{r} \|D^r g\|_\infty \|D^{\alpha-r} \phi\|_\infty \leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} \sum_{r=0}^{\alpha} \alpha^\alpha \|D^r g\|_\infty \frac{\sqrt{(\alpha-r)!}}{\sqrt{2\pi}} \\ &\leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} K \alpha^\alpha \frac{\sqrt{\alpha!}}{\sqrt{2\pi}} \leq K (\lfloor \beta \rfloor + 1)^{\lfloor \beta \rfloor + 1} \frac{\sqrt{\lfloor \beta \rfloor!}}{\sqrt{2\pi}}. \end{aligned} \quad (32)$$

Similarly, we have

$$\sum_{\alpha=0}^{\lfloor \beta \rfloor} \|D^\alpha(g\phi')\|_\infty \leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} \sum_{r=0}^{\alpha} \binom{\alpha}{r} \|D^r g\|_\infty \|D^{\alpha-r+1} \phi\|_\infty \leq K (\lfloor \beta \rfloor + 1)^{\lfloor \beta \rfloor + 1} \frac{\sqrt{(\lfloor \beta \rfloor + 1)!}}{\sqrt{2\pi}}. \quad (33)$$

Let  $A = [a, b]$ . For any differentiable function  $h : A \subseteq \mathbb{R} \rightarrow \mathbb{R}$  and  $0 < \gamma \leq 1$ , we have

$$\begin{aligned} \sup_{\substack{x, y \in A \\ x \neq y}} \frac{|h(x) - h(y)|}{|x - y|^\gamma} &\leq \sup_{\substack{x, y \in A \\ x \neq y \\ |x - y| \leq 1}} \frac{|h(x) - h(y)|}{|x - y|^\gamma} + \sup_{\substack{x, y \in A \\ |x - y| \geq 1}} \frac{|h(x) - h(y)|}{|x - y|^\gamma} \\ &\leq \sup_{\substack{x, y \in A \\ x \neq y \\ |x - y| \leq 1}} \frac{|h(x) - h(y)|}{|x - y|} + \sup_{\substack{x, y \in A \\ |x - y| \geq 1}} |h(x) - h(y)| \leq \|h'\|_\infty + 2\|h\|_\infty. \end{aligned} \quad (34)$$

If  $\beta > 1$ , it follows that

$$\begin{aligned}
 & \frac{|(\mathbf{D}^{\lfloor \beta \rfloor}(g\phi))(x) - (\mathbf{D}^{\lfloor \beta \rfloor}(g\phi))(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \\
 &= \frac{\left| \sum_{\alpha=0}^{\lfloor \beta \rfloor} \binom{\lfloor \beta \rfloor}{\alpha} \{(\mathbf{D}^\alpha g)(x)(\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi)(x) - (\mathbf{D}^\alpha g)(y)(\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi)(y)\} \right|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \\
 &\leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} \binom{\lfloor \beta \rfloor}{\alpha} |(\mathbf{D}^\alpha g)(x)| \left( \frac{|(\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi)(x) - (\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi)(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \right) \\
 &\quad + \sum_{\alpha=0}^{\lfloor \beta \rfloor} \binom{\lfloor \beta \rfloor}{\alpha} |(\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi)(y)| \left( \frac{|(\mathbf{D}^\alpha g)(x) - (\mathbf{D}^\alpha g)(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \right) \\
 &\leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} \binom{\lfloor \beta \rfloor}{\alpha} \|D^\alpha g\|_\infty \left( \|\mathbf{D}^{\lfloor \beta \rfloor - \alpha + 1} \phi\|_\infty + 2 \|\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi\|_\infty \right) \\
 &\quad + \sum_{\alpha=0}^{\lfloor \beta \rfloor - 1} \binom{\lfloor \beta \rfloor}{\alpha} \|\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi\|_\infty \left( \|\mathbf{D}^{\alpha+1} g\|_\infty + 2 \|D^\alpha g\|_\infty \right) \\
 &\quad + \|\phi\|_\infty \left( \frac{|(\mathbf{D}^{\lfloor \beta \rfloor} g)(x) - (\mathbf{D}^{\lfloor \beta \rfloor} g)(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \right)
 \end{aligned}$$

for any  $x, y \in A$  with  $x \neq y$ , where the last inequality holds by (34). Combining (31) with the last display, we have

$$\begin{aligned}
 & \sup_{\substack{x, y \in A \\ x \neq y}} \frac{|(\mathbf{D}^{\lfloor \beta \rfloor}(g\phi))(x) - (\mathbf{D}^{\lfloor \beta \rfloor}(g\phi))(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \\
 &\leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} \binom{\lfloor \beta \rfloor}{\alpha} \|D^\alpha g\|_\infty \left( \|\mathbf{D}^{\lfloor \beta \rfloor - \alpha + 1} \phi\|_\infty + 2 \|\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi\|_\infty \right) \\
 &\quad + \sum_{\alpha=0}^{\lfloor \beta \rfloor - 1} \binom{\lfloor \beta \rfloor}{\alpha} \|\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi\|_\infty \left( \|\mathbf{D}^{\alpha+1} g\|_\infty + 2 \|D^\alpha g\|_\infty \right) \\
 &\quad + \|\phi\|_\infty \left( \sup_{\substack{x, y \in A \\ x \neq y}} \frac{|(\mathbf{D}^{\lfloor \beta \rfloor} g)(x) - (\mathbf{D}^{\lfloor \beta \rfloor} g)(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \right) \\
 &\leq \sum_{\alpha=0}^{\lfloor \beta \rfloor} \binom{\lfloor \beta \rfloor}{\alpha} \|D^\alpha g\|_\infty \left( \frac{\sqrt{(\lfloor \beta \rfloor - \alpha + 1)!}}{\sqrt{2\pi}} + \frac{2\sqrt{(\lfloor \beta \rfloor - \alpha)!}}{\sqrt{2\pi}} \right) \\
 &\quad + \sum_{\alpha=0}^{\lfloor \beta \rfloor - 1} \binom{\lfloor \beta \rfloor}{\alpha} \|\mathbf{D}^{\lfloor \beta \rfloor - \alpha} \phi\|_\infty \left( \|\mathbf{D}^{\alpha+1} g\|_\infty + 2 \|D^\alpha g\|_\infty \right) \left( \frac{\sqrt{(\lfloor \beta \rfloor - \alpha)!}}{\sqrt{2\pi}} \right) \\
 &\quad + \frac{1}{\sqrt{2\pi}} \left( \sup_{\substack{x, y \in A \\ x \neq y}} \frac{|(\mathbf{D}^{\lfloor \beta \rfloor} g)(x) - (\mathbf{D}^{\lfloor \beta \rfloor} g)(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} \right).
 \end{aligned}$$

Moreover, the last display is bounded by

$$\begin{aligned}
 &\leq 3[\beta]^{|\beta|} \left( \frac{\sqrt{([\beta] + 1)!}}{\sqrt{2\pi}} \right) \left( \sum_{\alpha=0}^{[\beta]} \|D^\alpha g\|_\infty \right) \\
 &\quad + 3[\beta]^{|\beta|-1} \left( \frac{\sqrt{[\beta]!}}{\sqrt{2\pi}} \right) \left( \sum_{\alpha=0}^{[\beta]} \|D^\alpha g\|_\infty + \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|(D^{[\beta]}g)(x) - (D^{[\beta]}g)(y)|}{|x - y|^{\beta-[\beta]}} \right) \\
 &\leq 6K[\beta]^{|\beta|} \left( \frac{\sqrt{([\beta] + 1)!}}{\sqrt{2\pi}} \right). \tag{35}
 \end{aligned}$$

Similarly, we have

$$\begin{aligned}
 &\sup_{\substack{x,y \in A \\ x \neq y}} \frac{|(D^{[\beta]}(g\phi'))(x) - (D^{[\beta]}(g\phi'))(y)|}{|x - y|^{\beta-[\beta]}} \\
 &\leq \sum_{\alpha=0}^{[\beta]} \binom{[\beta]}{\alpha} \|D^\alpha g\|_\infty \left( \|D^{[\beta]-\alpha+2}\phi\|_\infty + 2\|D^{[\beta]-\alpha+1}\phi\|_\infty \right) \\
 &\quad + \sum_{\alpha=0}^{[\beta]-1} \binom{[\beta]}{\alpha} \|D^{[\beta]-\alpha+1}\phi\|_\infty \left( \|D^{\alpha+1}g\|_\infty + 2\|D^\alpha g\|_\infty \right) \\
 &\quad + \|\phi'\|_\infty \left( \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|(D^{[\beta]}g)(x) - (D^{[\beta]}g)(y)|}{|x - y|^{\beta-[\beta]}} \right) \\
 &\leq \sum_{\alpha=0}^{[\beta]} [\beta]^\alpha \|D^\alpha g\|_\infty \left( \frac{\sqrt{([\beta] - \alpha + 2)!}}{\sqrt{2\pi}} + \frac{2\sqrt{([\beta] - \alpha + 1)!}}{\sqrt{2\pi}} \right) \\
 &\quad + \sum_{\alpha=0}^{[\beta]-1} [\beta]^\alpha \left( \|D^{\alpha+1}g\|_\infty + 2\|D^\alpha g\|_\infty \right) \left( \frac{\sqrt{([\beta] - \alpha + 1)!}}{\sqrt{2\pi}} \right) \\
 &\quad + \frac{1}{\sqrt{2\pi}} \left( \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|(D^{[\beta]}g)(x) - (D^{[\beta]}g)(y)|}{|x - y|^{\beta-[\beta]}} \right) \\
 &\leq 6K[\beta]^{|\beta|} \left( \frac{\sqrt{([\beta] + 2)!}}{\sqrt{2\pi}} \right). \tag{36}
 \end{aligned}$$

If  $0 < \beta \leq 1$ , we have

$$\begin{aligned}
 \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|(g\phi)(x) - (g\phi)(y)|}{|x-y|^\beta} &\leq \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|g(x)\phi(x) - g(x)\phi(y) + g(x)\phi(y) - g(y)\phi(y)|}{|x-y|^\beta} \\
 &\leq \|g\|_\infty \left( \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|\phi(x) - \phi(y)|}{|x-y|^\beta} \right) + \|\phi\|_\infty \left( \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|g(x) - g(y)|}{|x-y|^\beta} \right) \\
 &\leq \left( \|g\|_\infty + \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|g(x) - g(y)|}{|x-y|^\beta} \right) (\|\phi'\|_\infty + 2\|\phi\|_\infty) \leq \frac{3K}{\sqrt{2\pi}}
 \end{aligned}$$

and

$$\begin{aligned}
 \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|(g\phi')(x) - (g\phi')(y)|}{|x-y|^\beta} &\leq \left( \|g\|_\infty + \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|g(x) - g(y)|}{|x-y|^\beta} \right) (\|\phi''\|_\infty + 2\|\phi'\|_\infty) \\
 &\leq \frac{3\sqrt{2}K}{\sqrt{2\pi}},
 \end{aligned}$$

where the second and third inequality holds by (34) and (31), respectively. Combining (32), (33), (35), (36) with the last display, we have  $g\phi \in \mathcal{H}_1^{\beta, KD_1}(A)$  and  $g\phi' \in \mathcal{H}_1^{\beta, KD_1}$ , where

$$D_1 = (\lfloor \beta \rfloor + 1)^{\lfloor \beta \rfloor + 1} \frac{\sqrt{(\lfloor \beta \rfloor + 1)!}}{\sqrt{2\pi}} + 6\lfloor \beta \rfloor^{\lfloor \beta \rfloor} \left( \frac{\sqrt{(\lfloor \beta \rfloor + 2)!}}{\sqrt{2\pi}} \right).$$

The assertion follows by re-defining the constant. ■

### B.1.3 PROOF OF LEMMA 22

**Proof** Consider  $\tau_{\text{bd}}, \tau_{\text{tail}} > 0, m \in n_\beta \mathbb{N}$  and real-valued  $D$ -dimensional vectors  $\mathbf{x} = (x_1, \dots, x_D)^\top, \mathbf{y} = (y_1, \dots, y_D)^\top$  such that  $\|\mathbf{x}\|_\infty \leq \mu - \mu\{\log(1/\sigma)\}^{-\tau_{\text{bd}}}$  and  $\|\mathbf{x} + \sigma\mathbf{y}\|_\infty \leq \mu$ . Let  $\mathbf{y}_{<i+1} = (y_1, \dots, y_i)^\top \in \mathbb{R}^i$  and  $\mathbf{y}_{>D-i} = (y_{D-i+1}, \dots, y_D)^\top \in \mathbb{R}^i$  for  $i \in [D]$ . For  $y \in \mathbb{R}$  and each  $i$ , denote  $(\mathbf{y}_{<i}, y, \mathbf{y}_{>i})$  as a  $D$ -dimensional vector that is identical to  $\mathbf{y}$  except for the  $i$ -th component, which is replaced by  $y$ .

Let  $D_\sigma = 2\sqrt{2\tau_{\text{tail}}}\{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})}$  and fix  $i \in [D]$ . Then,

$$-x_i - \mu \leq -\mu\{\log(1/\sigma)\}^{-\tau_{\text{bd}}} < 0 \quad \text{and} \quad -x_i + \mu \geq \mu\{\log(1/\sigma)\}^{-\tau_{\text{bd}}} > 0.$$

Moreover,  $(-x_i - \mu)/\sigma < (-x_i - \mu)D_\sigma < 0$  and  $(-x_i + \mu)/\sigma > (-x_i + \mu)D_\sigma > 0$  for small enough  $\sigma$  so that  $0 < D_\sigma \leq (2\sigma)^{-1}$ . Consider a one-dimensional real-valued function  $g_i$  such that

$$g_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) = p_0 \left( \frac{\mathbf{x} + \sigma(\mathbf{y}_{<i}, y, \mathbf{y}_{>i})}{\mu} \right) \phi(y), \quad y \in [(-x_i - \mu)/\sigma, (-x_i + \mu)/\sigma].$$

Then,

$$\begin{aligned}
 & \left| \int_{\frac{-x_i-\mu}{\sigma}}^{\frac{-x_i+\mu}{\sigma}} g_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy - \int_{(-x_i-\mu)D_\sigma}^{(-x_i+\mu)D_\sigma} g_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy \right| \\
 &= \int_{\frac{-x_i-\mu}{\sigma}}^{(-x_i-\mu)D_\sigma} g_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy + \int_{(-x_i+\mu)D_\sigma}^{\frac{-x_i+\mu}{\sigma}} g_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy \\
 &\leq K \int_{-\infty}^{(-x_i-\mu)D_\sigma} \phi(y) dy + K \int_{(-x_i+\mu)D_\sigma}^{\infty} \phi(y) dy \\
 &\leq K \exp\left(-\frac{(-x_i-\mu)^2 D_\sigma^2}{2}\right) + K \exp\left(-\frac{(-x_i+\mu)^2 D_\sigma^2}{2}\right) \\
 &\leq 2K \exp(-\tau_{\text{tail}} \log(1/\sigma)) = 2K \sigma^{\tau_{\text{tail}}},
 \end{aligned} \tag{37}$$

where the second inequality holds by the tail probability of the standard normal distribution. Let  $C_{G,1} = C_{G,1}(\beta)$  be the constant in Lemma 21. Since  $\sigma/\mu < 1$  for  $\sigma < 2$ , Lemma 21 implies that  $g_i \in \mathcal{H}_1^{\beta, KC_{G,1}}([(-x_i-\mu)D_\sigma, (-x_i+\mu)D_\sigma])$ . Moreover, Lemma 20 implies that

$$\begin{aligned}
 & \left| \int_{(-x_i-\mu)D_\sigma}^{(-x_i+\mu)D_\sigma} g_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy - \sum_{j=1}^m \tilde{v}_j g_i(\tilde{y}_j^{(i)}; \mathbf{y}_{<i}, \mathbf{y}_{>i}) \right| \\
 &\leq \left\{ \frac{2^{[\beta]+1} n_\beta^\beta}{[\beta]!} \right\} C_{G,1} K \mu^{\beta+1} D_\sigma^{\beta+1} m^{-\beta},
 \end{aligned} \tag{38}$$

where

$$\begin{aligned}
 \tilde{y}_j^{(i)} &= (-x_i - \mu)D_\sigma + \frac{\mu D_\sigma n_\beta}{m} \left\{ \tilde{x}_{j-n_\beta \lfloor \frac{j}{n_\beta} \rfloor} + 2 \left\lfloor \frac{j}{n_\beta} \right\rfloor + 1 \right\}, \\
 \tilde{v}_j &= \frac{\mu D_\sigma n_\beta}{m} \tilde{w}_{j-n_\beta \lfloor \frac{j}{n_\beta} \rfloor},
 \end{aligned}$$

and  $(-x_i - \mu)D_\sigma < \tilde{y}_j^{(i)} < (-x_i + \mu)D_\sigma$  for  $j \in [m]$ . Combining (37) and (38), we have

$$\left| \int_{\frac{-x_i-\mu}{\sigma}}^{\frac{-x_i+\mu}{\sigma}} p_0\left(\frac{\mathbf{x} + \sigma(\mathbf{y}_{<i}, y, \mathbf{y}_{>i})}{\mu}\right) \phi(y) dy - \sum_{j=1}^m \tilde{v}_j g_i(\tilde{y}_j^{(i)}; \mathbf{y}_{<i}, \mathbf{y}_{>i}) \right| \leq \epsilon, \tag{39}$$

where  $\epsilon = 2K \sigma^{\tau_{\text{tail}}} + 2^{[\beta]+1} n_\beta^\beta C_{G,1} K \mu^{\beta+1} D_\sigma^{\beta+1} m^{-\beta} / [\beta]!$ . Since  $|x_i| \leq \mu - \mu \{\log(1/\sigma)\}^{-\tau_{\text{bd}}}$  and  $\sigma D_\sigma \leq 1/2$ , we have

$$\frac{x_i}{2\mu} - \frac{1}{2} \leq \frac{x_i + \sigma D_\sigma (-x_i - \mu)}{\mu} \leq \frac{x_i + \sigma \tilde{y}_j^{(i)}}{\mu} \leq \frac{x_i + \sigma D_\sigma (-x_i + \mu)}{\mu} \leq \frac{x_i}{2\mu} + \frac{1}{2}$$

and

$$\left| \frac{x_i + \sigma \tilde{y}_j^{(i)}}{\mu} \right| \leq 1 - \frac{\{\log(1/\sigma)\}^{-\tau_{\text{bd}}}}{2} < 1.$$

Consider  $F_{(j_1), \dots, (j_1, \dots, j_D)}$  for  $j_1, \dots, j_D \in [m]$ , defined as

$$F_{(j_1, \dots, j_{k-1})} = \int_{\|\mathbf{x}_{>k} + \sigma \mathbf{y}_{>k}\|_\infty \leq \mu} \left\{ \int_{\frac{-x_k - \mu}{\sigma}}^{\frac{-x_k + \mu}{\sigma}} p_0 \left( \frac{\mathbf{x} + \sigma \left( \tilde{y}_{j_1}^{(1)}, \dots, \tilde{y}_{j_{k-1}}^{(k-1)}, y, \mathbf{y}_{>k}^\top \right)^\top}{\mu} \right) \phi(y) dy \right\} \prod_{i=k+1}^D \phi(y_i) d\mathbf{y}_{>k},$$

for  $k \in \{2, \dots, D-1\}$ ,

$$F_{(j_1, \dots, j_{D-1})} = \int_{\frac{-x_D - \mu}{\sigma}}^{\frac{-x_D + \mu}{\sigma}} p_0 \left( \frac{\mathbf{x} + \sigma \left( \tilde{y}_{j_1}^{(1)}, \dots, \tilde{y}_{j_{D-1}}^{(D-1)}, y \right)^\top}{\mu} \right) \phi(y) dy, \quad \text{and}$$

$$F_{(j_1, \dots, j_D)} = p_0 \left( \frac{\mathbf{x} + \sigma \left( \tilde{y}_{j_1}^{(1)}, \dots, \tilde{y}_{j_D}^{(D)} \right)^\top}{\mu} \right).$$

For any  $k \in \{2, \dots, D-1\}$  and  $j_1, \dots, j_D \in [m]$ , we have

$$\begin{aligned} & \left| F_{(j_1, \dots, j_{k-1})} - \sum_{j_k=1}^m \tilde{v}_{j_k} \phi \left( \tilde{y}_{j_k}^{(k)} \right) F_{(j_1, \dots, j_k)} \right| \\ & \leq \epsilon \int_{\|\mathbf{x}_{>k} + \sigma \mathbf{y}_{>k}\|_\infty \leq \mu} \left\{ \prod_{i=k+1}^D \phi(y_i) \right\} d\mathbf{y}_{>k} \leq \epsilon \end{aligned} \quad (40)$$

and

$$\left| F_{(j_1, \dots, j_{D-1})} - \sum_{j_D=1}^m \tilde{v}_{j_D} \phi \left( \tilde{y}_{j_D}^{(D)} \right) F_{(j_1, \dots, j_D)} \right| \leq \epsilon,$$

where the first and last inequality holds by (39). Note that

$$\mu^D p_{\mu, \sigma}(\mathbf{x}) = \int_{\|\mathbf{x}_{>1} + \sigma \mathbf{y}_{>1}\|_\infty \leq \mu} \left[ \int_{\frac{-x_1 - \mu}{\sigma}}^{\frac{-x_1 + \mu}{\sigma}} \left\{ p_0 \left( \frac{\mathbf{x} + \sigma (y, \mathbf{y}_{>1}^\top)^\top}{\mu} \right) \phi(y) \right\} dy \right] \prod_{i=2}^D \phi(y_i) d\mathbf{y}_{>1}.$$

Then, we also have

$$\left| \mu^D p_{\mu, \sigma}(\mathbf{x}) - \sum_{j_1=1}^m \tilde{v}_{j_1} \phi \left( \tilde{y}_{j_1}^{(1)} \right) F_{(j_1)} \right| \leq \epsilon \int_{\|\mathbf{x}_{>1} + \sigma \mathbf{y}_{>1}\|_\infty \leq \mu} \left\{ \prod_{i=2}^D \phi(y_i) \right\} d\mathbf{y}_{>1} \leq \epsilon,$$

where the first inequality holds by (39). Combining (40) with the last display, we have

$$\begin{aligned}
 & \left| \mu^D p_{\mu, \sigma}(\mathbf{x}) - \sum_{j_1, \dots, j_D=1}^m \prod_{k=1}^D \left\{ \tilde{v}_{j_k} \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} F_{(j_1, \dots, j_D)} \right| \\
 & \leq \left| \mu^D p_{\mu, \sigma}(\mathbf{x}) - \sum_{j_1=1}^m \tilde{v}_{j_1} \phi \left( \tilde{y}_{j_1}^{(1)} \right) F_{(j_1)} \right| \\
 & \quad + \sum_{i=2}^D \left| \sum_{j_1, \dots, j_{i-1}=1}^m \prod_{k=1}^{i-1} \left\{ \tilde{v}_{j_k} \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} \left\{ F_{(j_1, \dots, j_{i-1})} - \sum_{j_i=1}^m \tilde{v}_{j_i} \phi \left( \tilde{y}_{j_i}^{(i)} \right) F_{(j_1, \dots, j_i)} \right\} \right| \quad (41) \\
 & \leq \epsilon \left( 1 + \sum_{i=2}^D \sum_{j_1, \dots, j_{i-1}=1}^m \left| \prod_{k=1}^{i-1} \left\{ \tilde{v}_{j_k} \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} \right| \right) \\
 & \leq \epsilon \left( 1 + \sum_{i=2}^D \sum_{j_1, \dots, j_{i-1}=1}^m \frac{\left| \prod_{k=1}^{i-1} \tilde{v}_{j_k} \right|}{(2\pi)^{\frac{i-1}{2}}} \right),
 \end{aligned}$$

where the last inequality holds because  $|\phi| \leq 1/\sqrt{2\pi}$ . For each  $j \in [m]$ , we have

$$|\tilde{v}_j| \leq \left\{ \frac{\mu D_\sigma n_\beta}{m} \right\} \max(|\tilde{w}_1|, \dots, |\tilde{w}_{n_\beta}|) = \frac{D_1 \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})}}{m},$$

where the last inequality holds because  $\mu \leq 1$  and  $D_1 = 2\sqrt{2\tau_{\text{tail}}} n_\beta \max(|\tilde{w}_1|, \dots, |\tilde{w}_{n_\beta}|)$ . Then,

$$\begin{aligned}
 & 1 + \sum_{i=2}^D \sum_{j_1, \dots, j_{i-1}=1}^m \frac{\left| \prod_{k=1}^{i-1} \tilde{v}_{j_k} \right|}{(2\pi)^{\frac{i-1}{2}}} \leq 1 + \sum_{i=2}^D \sum_{j_1, \dots, j_{i-1}=1}^m \left( \frac{D_1 \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})}}{m\sqrt{2\pi}} \right)^{i-1} \\
 & = 1 + \sum_{i=2}^D \left( \frac{D_1 \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})}}{\sqrt{2\pi}} \right)^{i-1} \leq D \left( \frac{D_1 \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})}}{\sqrt{2\pi}} \right)^{D-1},
 \end{aligned}$$

where the last inequality holds for small enough  $\sigma$  so that  $D_1 \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})} \geq \sqrt{2\pi}$ . Also, there exists a constant  $D_2 = D_2(\beta, \tau_{\text{tail}}, C_{G,1})$  such that

$$\epsilon \leq D_2 K \left( \sigma^{\tau_{\text{tail}}} + m^{-\beta} \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})(\beta+1)} \right).$$

Hence,

$$\begin{aligned}
 & \left| \mu^D p_{\mu, \sigma}(\mathbf{x}) - \sum_{j_1, \dots, j_D=1}^m \prod_{k=1}^D \left\{ \tilde{v}_{j_k} \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} F_{(j_1, \dots, j_D)} \right| \\
 & \leq \epsilon \left( 1 + \sum_{i=2}^D \sum_{j_1, \dots, j_{i-1}=1}^m \frac{\left| \prod_{k=1}^{i-1} \tilde{v}_{j_k} \right|}{(2\pi)^{\frac{i-1}{2}}} \right) \quad (42) \\
 & \leq D_3 K \left( \sigma^{\tau_{\text{tail}}} + m^{-\beta} \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})(\beta+1)} \right) \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})(D-1)},
 \end{aligned}$$

where  $D_3 = DD_2(D_1/\sqrt{2\pi})^{D-1}$ .

Note that

$$\begin{aligned}\nabla p_{\mu,\sigma}(\mathbf{x}) &= \int_{\|\mathbf{y}\|_\infty \leq 1} \left( \frac{\mu\mathbf{y} - \mathbf{x}}{\sigma^2} \right) p_0(\mathbf{y}) \phi_\sigma(\mathbf{x} - \mu\mathbf{y}) d\mathbf{y} \\ &= \sigma^{-1} \mu^{-D} \int_{\|\mathbf{x} + \sigma\mathbf{y}\|_\infty \leq \mu} (y_1, \dots, y_D)^\top p_0 \left( \frac{\mathbf{x} + \sigma\mathbf{y}}{\mu} \right) \prod_{i=1}^D \phi(y_i) d\mathbf{y}.\end{aligned}$$

For  $i \in [D]$ , consider a one-dimensional real-valued function  $\tilde{g}_i$  such that

$$\tilde{g}_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) = yg_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}), \quad y \in [(-x_i - \mu)/\sigma, (-x_i + \mu)/\sigma].$$

Then,

$$\begin{aligned}& \left| \int_{\frac{-x_i - \mu}{\sigma}}^{\frac{-x_i + \mu}{\sigma}} \tilde{g}_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy - \int_{(-x_i - \mu)D_\sigma}^{(-x_i + \mu)D_\sigma} \tilde{g}_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy \right| \\ & \leq \left| \int_{\frac{-x_i - \mu}{\sigma}}^{(-x_i - \mu)D_\sigma} \tilde{g}_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy \right| + \left| \int_{(-x_i + \mu)D_\sigma}^{\frac{-x_i + \mu}{\sigma}} \tilde{g}_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy \right| \\ & \leq K \int_{(x_i + \mu)D_\sigma}^{\infty} y\phi(y) dy + K \int_{(-x_i + \mu)D_\sigma}^{\infty} y\phi(y) dy \\ & = K \exp\left(-\frac{(x_i + \mu)^2 D_\sigma^2}{2}\right) + K \exp\left(-\frac{(-x_i + \mu)^2 D_\sigma^2}{2}\right) \\ & \leq 2K \exp(-\tau_{\text{tail}} \log(1/\sigma)) = 2K\sigma^{\tau_{\text{tail}}},\end{aligned} \tag{43}$$

where the first equality holds because

$$-x_i - \mu \leq -\{\log(1/\sigma)\}^{-\tau_{\text{bd}}}/2 < 0 \quad \text{and} \quad -x_i + \mu \geq 2^{-1}\{\log(1/\sigma)\}^{-\tau_{\text{bd}}} > 0.$$

Since  $\phi'(y) = -y\phi(y)$  for  $y \in \mathbb{R}$  and  $\sigma/\mu < 1$ , Lemma 21 implies that  $\tilde{g}_i \in \mathcal{H}_1^{\beta, KCG, 1}((-x_i - \mu)D_\sigma, (-x_i + \mu)D_\sigma]$ . Moreover, Lemma 20 implies that

$$\begin{aligned}& \left| \int_{(-x_i - \mu)D_\sigma}^{(-x_i + \mu)D_\sigma} \tilde{g}_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) dy - \sum_{j=1}^m \tilde{v}_j \tilde{y}_j^{(i)} g_i(\tilde{y}_j^{(i)}; \mathbf{y}_{<i}, \mathbf{y}_{>i}) \right| \\ & \leq \left\{ \frac{2^{[\beta]+1} n \beta^\beta}{[\beta]!} \right\} C_{G,1} K \mu^{\beta+1} D_\sigma^{\beta+1} m^{-\beta}\end{aligned}$$

because  $\tilde{g}_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i}) = yg_i(y; \mathbf{y}_{<i}, \mathbf{y}_{>i})$ . Combining (43) with the last display, we have

$$\left| \int_{\frac{-x_i - \mu}{\sigma}}^{\frac{-x_i + \mu}{\sigma}} p_0 \left( \frac{\mathbf{x} + \sigma(\mathbf{y}_{<i}, y, \mathbf{y}_{>i})}{\mu} \right) y\phi(y) dy - \sum_{j=1}^m \tilde{v}_j \tilde{y}_j^{(i)} g_i(\tilde{y}_j^{(i)}; \mathbf{y}_{<i}, \mathbf{y}_{>i}) \right| \leq \epsilon. \tag{44}$$

Combining (39) with a simple calculation, we have

$$\begin{aligned}
 & \left| \int_{\|\mathbf{x}-i+\sigma\mathbf{y}-i\|_\infty \leq \mu} p_0 \left( \frac{\mathbf{x} + \sigma(\mathbf{y}_{<i}, y, \mathbf{y}_{>i})}{\mu} \right) \prod_{\substack{k=1 \\ k \neq i}}^D \phi(y_k) d\mathbf{y}_{<i} \right. \\
 & \quad \left. - \sum_{\substack{j_1, \dots, j_D=1 \\ \text{w/o } j_i}}^m \prod_{\substack{k=1 \\ k \neq i}}^D \left\{ \tilde{v}_{j_k} \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} p_0 \left( \frac{\mathbf{x} + \sigma \left( \tilde{y}_{j_1}^{(1)}, \dots, \tilde{y}_{j_{i-1}}^{(i-1)}, y, \tilde{y}_{j_{i+1}}^{(i+1)}, \dots, \tilde{y}_{j_D}^{(D)} \right)^\top}{\mu} \right) \right| \\
 & \leq \epsilon \left( 1 + \sum_{h=1}^{D-1} \sum_{\substack{j_1, \dots, j_h=1 \\ \text{w/o } j_i}}^m \prod_{\substack{k=1 \\ k \neq i}}^h \left\{ |\tilde{v}_{j_k}| \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} \right)
 \end{aligned}$$

for any  $y \in \mathbb{R}$  satisfying  $|x_i + \sigma y| \leq \mu$ , where  $\sum_{j_1, \dots, j_D=1}^m \text{w/o } j_i$  denotes the summation over  $1 \leq j_1, \dots, j_{i-1}, j_{i+1}, \dots, j_D \leq m$ .

Note that

$$\begin{aligned}
 \mu^D \sigma (\nabla p_{\mu, \sigma}(\mathbf{x}))_i &= \int_{\|\mathbf{x} + \sigma\mathbf{y}\|_\infty \leq \mu} y_i p_0 \left( \frac{\mathbf{x} + \sigma\mathbf{y}}{\mu} \right) \prod_{k=1}^D \phi(y_k) d\mathbf{y} \\
 &= \int_{\frac{-x_i - \mu}{\sigma}}^{\frac{-x_i + \mu}{\sigma}} \left\{ \int_{\|\mathbf{x}-i+\sigma\mathbf{y}-i\|_\infty \leq \mu} p_0 \left( \frac{\mathbf{x} + \sigma\mathbf{y}}{\mu} \right) \prod_{\substack{k=1 \\ k \neq i}}^D \phi(y_k) d\mathbf{y}_{<i} \right\} y_i \phi(y_i) dy_i.
 \end{aligned}$$

Combining (44) with the last three displays, we have

$$\begin{aligned}
 & \left| \int_{\|\mathbf{x} + \sigma\mathbf{y}\|_\infty \leq \mu} y_i p_0 \left( \frac{\mathbf{x} + \sigma\mathbf{y}}{\mu} \right) \prod_{k=1}^D \phi(y_k) d\mathbf{y} - \sum_{j_1, \dots, j_D=1}^m \tilde{y}_{j_i}^{(i)} \prod_{k=1}^D \left\{ \tilde{v}_{j_k} \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} F_{(j_1, \dots, j_D)} \right| \\
 & \leq \epsilon \left( 1 + \sum_{h=1}^{D-1} \sum_{\substack{j_1, \dots, j_h=1 \\ \text{w/o } j_i}}^m \prod_{\substack{k=1 \\ k \neq i}}^h \left\{ |\tilde{v}_{j_k}| \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} + \sum_{\substack{j_1, \dots, j_D=1 \\ \text{w/o } j_i}}^m \prod_{\substack{k=1 \\ k \neq i}}^D \left\{ |\tilde{v}_{j_k}| \phi \left( \tilde{y}_{j_k}^{(k)} \right) \right\} \right) \int_{\frac{-x_i - \mu}{\sigma}}^{\frac{-x_i + \mu}{\sigma}} |y| \phi(y) dy \\
 & \leq \frac{2\epsilon}{\sqrt{2\pi}} \left( 1 + \sum_{h=1}^D \sum_{\substack{j_1, \dots, j_h=1 \\ \text{w/o } j_i}}^m \prod_{\substack{k=1 \\ k \neq i}}^h \frac{|\tilde{v}_{j_k}|}{\sqrt{2\pi}} \right),
 \end{aligned}$$

where the last inequality holds because  $\int_{-\infty}^{\infty} |y| \phi(y) dy = 2 \int_0^{\infty} y \phi(y) dy = \frac{2}{\sqrt{2\pi}}$  and  $|\phi| \leq 1/\sqrt{2\pi}$ . Combining with (42), the last display is bounded by

$$\frac{2D_3 K}{\sqrt{2\pi}} \left( \sigma^{\tau_{\text{tail}}} + m^{-\beta} \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})(\beta+1)} \right) \{\log(1/\sigma)\}^{(\tau_{\text{bd}} + \frac{1}{2})(D-1)},$$

and the assertion follows by re-defining constants.  $\blacksquare$

## B.2 Proof of Proposition 23

**Proof** Let  $\delta > 0$  be a small enough value as described below. There exists neural networks  $f_\mu \in \mathcal{F}_{\text{NN}}(L_\mu, \mathbf{d}_\mu, s_\mu, M_\mu)$ ,  $f_\sigma \in \mathcal{F}_{\text{NN}}(L_\sigma, \mathbf{d}_\sigma, s_\sigma, M_\sigma)$  with

$$\begin{aligned} L_\mu, L_\sigma &\leq C_{N,4} \{\log(1/\delta)\}^2, & \|\mathbf{d}_\mu\|_\infty, \|\mathbf{d}_\sigma\|_\infty &\leq C_{N,4} \{\log(1/\delta)\}^2 \\ s_\mu, s_\sigma &\leq C_{N,4} \{\log(1/\delta)\}^3, & M_\mu, M_\sigma &\leq C_{N,4} \log(1/\delta) \end{aligned}$$

such that

$$|\mu_t - f_\mu(t)| \leq \delta \quad \text{and} \quad |\sigma_t - f_\sigma(t)| \leq \delta \quad (45)$$

for  $t \geq \delta$ , where  $C_{N,4}$  is the constant in Lemma 18. for any  $0 \leq t \leq (2\bar{\tau})^{-1}$ .

Since  $\log(1/x) = -\log x$  for any  $x > 0$ , Lemma 16 implies that there exists a positive constant  $D_1 = D_1(\bar{\tau})$  and neural network  $f_{\log} \in \mathcal{F}_{\text{NN}}(L_{\log}, \mathbf{d}_{\log}, s_{\log}, M_{\log})$  with

$$\begin{aligned} L_{\log} &\leq D_1 \{\log(1/\delta)\}^2 \log \log(1/\delta), & \|\mathbf{d}_{\log}\|_\infty &\leq D_1 \{\log(1/\delta)\}^3 \\ s_{\log} &\leq D_1 \{\log(1/\delta)\}^5 \log \log(1/\delta), & M_{\log} &\leq \exp(D_1 \{\log(1/\delta)\}^2) \end{aligned}$$

such that  $|\log(1/x) - f_{\log}(\tilde{x})| \leq \sqrt{\bar{\tau}\delta}/2 + (2/\sqrt{\bar{\tau}\delta})|x - \tilde{x}|$  for  $\sqrt{\bar{\tau}\delta}/2 \leq x \leq (\sqrt{\bar{\tau}\delta}/2)^{-1}$  and  $\tilde{x} \in \mathbb{R}$ . Combining with (45), we have

$$|\log(1/\sigma_t) - f_{\log}(f_\sigma(t))| \leq \frac{2\sqrt{\delta}}{\sqrt{\bar{\tau}}} + \frac{\sqrt{\bar{\tau}\delta}}{2} = \left( \frac{2}{\sqrt{\bar{\tau}}} + \frac{\sqrt{\bar{\tau}}}{2} \right) \sqrt{\delta} \quad (46)$$

for  $\delta \leq t \leq (2\bar{\tau})^{-1}$ . Let

$$\tau_{\text{mult}} = \tau_{\text{bd}} + 1$$

Lemma 14 implies that for  $k \geq 2$ , there exists a neural network  $f_{\text{mult}}^{(k)} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}^{(k)}, \mathbf{d}_{\text{mult}}^{(k)}, s_{\text{mult}}^{(k)}, M_{\text{mult}}^{(k)})$  with

$$\begin{aligned} L_{\text{mult}}^{(k)} &\leq C_{N,1} (k\tau_{\text{mult}} + 1) \log k \log(1/\delta), & \|\mathbf{d}_{\text{mult}}^{(k)}\|_\infty &= 48k, \\ s_{\text{mult}}^{(k)} &\leq C_{N,1} k (\tau_{\text{mult}} + 1) \log(1/\delta), & M_{\text{mult}}^{(k)} &= \{\log(1/\delta)\}^{k\tau_{\text{mult}}} \end{aligned}$$

such that

$$\left| f_{\text{mult}}^{(k)}(\tilde{x}_1, \dots, \tilde{x}_k) - \prod_{i=1}^k x_i \right| \leq \delta + k \{\log(1/\delta)\}^{(k-1)\tau_{\text{mult}}} \tilde{\epsilon} \quad (47)$$

for any  $\mathbf{x} = (x_1, \dots, x_k) \in \mathbb{R}^k$  with  $\|\mathbf{x}\|_\infty \leq \{\log(1/\delta)\}^{\tau_{\text{mult}}}$  and  $\tilde{\mathbf{x}} = (\tilde{x}_1, \dots, \tilde{x}_k) \in \mathbb{R}^k$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ , where  $0 < \tilde{\epsilon} \leq 1$  and  $C_{N,1}$  is the constant in Lemma 14. Combining Lemma 11 and Lemma 9 with the last display, there exists a neural network  $f_{\text{pow}}^{(k)} \in \mathcal{F}_{\text{NN}}(L_{\text{pow}}^{(k)}, \mathbf{d}_{\text{pow}}^{(k)}, s_{\text{pow}}^{(k)}, M_{\text{pow}}^{(k)})$  with

$$L_{\text{pow}}^{(k)} = L_{\text{mult}}^{(k)} + 2, \quad \|\mathbf{d}_{\text{pow}}^{(k)}\|_\infty \leq 96k, \quad s_{\text{pow}}^{(k)} \leq 2s_{\text{mult}}^{(k)} + 8k, \quad M_{\text{pow}}^{(k)} = M_{\text{mult}}^{(k)} \vee 1$$

such that

$$\left| f_{\text{pow}}^{(k)}(\tilde{x}) - x^k \right| \leq \delta + k \{\log(1/\delta)\}^{(k-1)\tau_{\text{mult}}}\tilde{\epsilon} \quad (48)$$

for any  $|x| \leq \{\log(1/\delta)\}^{\tau_{\text{mult}}}$  and  $\tilde{x} \in \mathbb{R}$  with  $|x - \tilde{x}| \leq \tilde{\epsilon}$ . For  $\delta \leq t \leq (2\bar{\tau})^{-1}$ , we have

$$|\log(1/\sigma_t)| \leq \log(1/\sqrt{\bar{\tau}\delta}) \leq \log(1/\delta), \quad (49)$$

where the first inequality holds by (27) and the last inequality holds with small enough  $\delta$ . Combining (46) with (48), it follows that

$$\begin{aligned} & \left| \{\log(1/\sigma_t)\}^{\tau_{\text{bd}}+\frac{1}{2}} - f_{\text{pow}}^{(\tau_{\text{bd}}+\frac{1}{2})}(f_{\log}(f_{\sigma}(t))) \right| \\ & \leq \delta + \left( \tau_{\text{bd}} + \frac{1}{2} \right) \left( \frac{2}{\sqrt{\bar{\tau}}} + \frac{\sqrt{\bar{\tau}}}{2} \right) \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}}-\frac{1}{2})\tau_{\text{mult}}} \\ & \leq D_2 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}}-\frac{1}{2})\tau_{\text{mult}}} \end{aligned} \quad (50)$$

for  $\delta \leq t \leq (2\bar{\tau})^{-1}$ , where  $D_2 = 1 + (\tau_{\text{bd}} + \frac{1}{2})(\frac{2}{\sqrt{\bar{\tau}}} + \frac{\sqrt{\bar{\tau}}}{2})$ . Combining (47) with the last two displays, we have

$$\begin{aligned} & \left| \{\log(1/\sigma_t)\}^{\tau_{\text{bd}}+\frac{1}{2}} x - f_{\text{mult}}^{(2)} \left( f_{\text{pow}}^{(\tau_{\text{bd}}+\frac{1}{2})}(f_{\log}(f_{\sigma}(t))), x \right) \right| \\ & \leq \delta + 2D_2 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}}+\frac{1}{2})\tau_{\text{mult}}} \leq D_3 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}}+\frac{1}{2})\tau_{\text{mult}}} \end{aligned}$$

for  $\delta \leq t \leq (2\bar{\tau})^{-1}$  and  $|x| \leq 1$ , where  $D_3 = 1 + 2D_2$ . Let  $m \in n_{\beta}\mathbb{N}$  be a large enough value as described below. Then, consider functions  $g_y^{(1)}, \dots, g_y^{(m)} : [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}$  and  $f_y^{(1)}, \dots, f_y^{(m)} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} & g_y^{(j)}(x, t) \\ & = 2\sqrt{2\tau_{\text{tail}}}\{\log(1/\sigma_t)\}^{\tau_{\text{bd}}+\frac{1}{2}} \left\{ -x - \mu_t + \frac{\mu_t n_{\beta}}{m} \left( \tilde{x}_{j-n_{\beta}\lfloor \frac{j}{n_{\beta}} \rfloor} + 2 \left\lfloor \frac{j}{n_{\beta}} \right\rfloor + 1 \right) \right\}, \quad j \in [m] \end{aligned}$$

for  $x \in [-1, 1], t \in [0, \infty)$  and

$$\begin{aligned} f_y^{(j)}(x, t) & = 2\sqrt{2\tau_{\text{tail}}} \left\{ -f_{\text{mult}}^{(2)} \left( f_{\text{pow}}^{(\tau_{\text{bd}}+\frac{1}{2})}(f_{\log}(f_{\sigma}(t))), x \right) - f_{\text{mult}}^{(2)} \left( f_{\text{pow}}^{(\tau_{\text{bd}}+\frac{1}{2})}(f_{\log}(f_{\sigma}(t))), f_{\mu}(t) \right) \right. \\ & \quad \left. + \frac{n_{\beta}}{m} \left( \tilde{x}_{j-n_{\beta}\lfloor \frac{j}{n_{\beta}} \rfloor} + 2 \left\lfloor \frac{j}{n_{\beta}} \right\rfloor + 1 \right) f_{\text{mult}}^{(2)} \left( f_{\text{pow}}^{(\tau_{\text{bd}}+\frac{1}{2})}(f_{\log}(f_{\sigma}(t))), f_{\mu}(t) \right) \right\}, \quad j \in [m] \end{aligned}$$

for  $x, t \in \mathbb{R}$ , where  $\{(\tilde{x}_j, \tilde{w}_j) : j \in [n_{\beta}]\}$  are the constants in Lemma 22. Then,

$$\begin{aligned} & \left| g_y^{(j)}(x, t) - f_y^{(j)}(x, t) \right| \\ & \leq 2\sqrt{2\tau_{\text{tail}}} \left\{ D_3 + \frac{D_3 n_{\beta}}{m} \left( \left| \tilde{x}_{j-n_{\beta}\lfloor \frac{j}{n_{\beta}} \rfloor} \right| + 2 \left\lfloor \frac{j}{n_{\beta}} \right\rfloor + 1 \right) + 1 \right\} \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}}+\frac{1}{2})\tau_{\text{mult}}} \end{aligned}$$

and

$$\left| g_y^{(j)}(x, t) \right| \leq 2\sqrt{2\tau_{\text{tail}}} \left\{ 2 + \frac{2n_{\beta}}{m} \left( \left| \tilde{x}_{j-n_{\beta}\lfloor \frac{j}{n_{\beta}} \rfloor} \right| + 2 \left\lfloor \frac{j}{n_{\beta}} \right\rfloor + 1 \right) \right\} \{\log(1/\delta)\}^{\tau_{\text{bd}}+\frac{1}{2}}$$

for  $|x| \leq 1$  and  $\delta \leq t \leq (4\bar{\tau})^{-1}$ , where the last inequality holds by (49). Then, there exists a constant  $D_4 = D_4(\beta, \tau_{\text{tail}}, \tau_{\text{bd}}, D_3)$  such that

$$\begin{aligned} \left| f_y^{(j)}(x, t) \right| &\leq \left| g_y^{(j)}(x, t) - f_y^{(j)}(x, t) \right| + \left| g_y^{(j)}(x, t) \right| \leq D_4 \{\log(1/\delta)\}^{\tau_{\text{bd}} + \frac{1}{2}}, \quad \text{and} \\ \left| g_y^{(j)}(x, t) - f_y^{(j)}(x, t) \right| &\leq D_4 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + \frac{1}{2})\tau_{\text{mult}}} \end{aligned} \quad (51)$$

for  $|x| \leq 1$  and  $\delta \leq t \leq (2\bar{\tau})^{-1}$  with small enough  $\delta$  so that  $\sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + \frac{1}{2})\tau_{\text{mult}}} \leq \{\log(1/\delta)\}^{\tau_{\text{bd}} + \frac{1}{2}}$ . Lemma 9 implies that  $f_{\text{pow}}^{(\tau_{\text{bd}} + \frac{1}{2})} \circ f_{\log} \circ f_{\sigma} \in \mathcal{F}_{\text{NN}}(L_{\text{pl}\sigma}, \mathbf{d}_{\text{pl}\sigma}, s_{\text{pl}\sigma}, M_{\text{pl}\sigma})$  with

$$\begin{aligned} L_{\text{pl}\sigma} &= L_{\text{pow}}^{(\tau_{\text{bd}} + \frac{1}{2})} + L_{\log} + L_{\sigma} \leq D_5 \{\log(1/\delta)\}^2 \log \log(1/\delta), \\ \|\mathbf{d}_{\text{pl}\sigma}\|_{\infty} &\leq 2 \max \left( \|\mathbf{d}_{\text{pow}}^{(\tau_{\text{bd}} + \frac{1}{2})}\|_{\infty}, \|\mathbf{d}_{\log}\|_{\infty}, \|\mathbf{d}_{\sigma}\|_{\infty} \right) \leq D_5 \{\log(1/\delta)\}^3, \\ s_{\text{pl}\sigma} &\leq 2 \left( s_{\text{pow}}^{(\tau_{\text{bd}} + \frac{1}{2})} + s_{\log} + s_{\sigma} \right) \leq D_5 \{\log(1/\delta)\}^5 \log \log(1/\delta), \\ M_{\text{pl}\sigma} &= \max \left( M_{\text{pow}}^{(\tau_{\text{bd}} + \frac{1}{2})}, M_{\log}, M_{\sigma} \right) \leq \exp \left( D_5 \{\log(1/\delta)\}^2 \right), \end{aligned}$$

where  $D_5 = D_5(\tau_{\text{bd}}, C_{N,1}, C_{N,4}, D_1)$ . Then, Lemma 9, Lemma 10 and Lemma 11 imply that  $f_y^{(j)} \in \mathcal{F}_{\text{NN}}(L_x, \mathbf{d}_x, s_x, M_x^{(j)})$  for  $j \in [m]$  with

$$\begin{aligned} L_x &\leq D_6 \{\log(1/\delta)\}^2 \log \log(1/\delta), \quad \|\mathbf{d}_x\|_{\infty} \leq D_6 \{\log(1/\delta)\}^3, \\ s_x &\leq D_6 \{\log(1/\delta)\}^5 \log \log(1/\delta), \quad M_x^{(j)} \leq \exp \left( D_6 \{\log(1/\delta)\}^2 \right), \end{aligned} \quad (52)$$

where  $D_6 = D_6(\beta, \tau_{\text{tail}}, C_{N,1}, C_{N,4}, D_3, D_5)$ . Let  $C_{N,5}$  be the constant in Lemma 19. Then, there exists a neural network  $f_{\text{rec}} \in \mathcal{F}_{\text{NN}}(L_{\text{rec}}, \mathbf{d}_{\text{rec}}, s_{\text{rec}}, M_{\text{rec}})$  with

$$\begin{aligned} L_{\text{rec}} &\leq C_{N,5} \{\log(1/\delta)\}^2, \quad \|\mathbf{d}_{\text{rec}}\|_{\infty} \leq C_{N,5} \{\log(1/\delta)\}^3 \\ s_{\text{rec}} &\leq C_{N,5} \{\log(1/\delta)\}^4, \quad M_{\text{rec}} \leq C_{N,5} \delta^{-2} \end{aligned}$$

such that  $|x^{-1} - f_{\text{rec}}(x)| \leq \delta$  for  $x \in [\delta, 1/\delta]$ . Combining with (45), we have

$$\begin{aligned} \left| \frac{1}{\mu_t} - f_{\text{rec}}(f_{\mu}(t)) \right| &\leq \left| \frac{1}{\mu_t} - \frac{1}{f_{\mu}(t)} \right| + \left| \frac{1}{f_{\mu}(t)} - f_{\text{rec}}(f_{\mu}(t)) \right| \\ &\leq (\mu_t \wedge f_{\mu}(t))^{-2} |\mu_t - f_{\mu}(t)| + \delta \leq 17\delta \end{aligned} \quad (53)$$

for  $\delta \leq t \leq (2\bar{\tau})^{-1}$ , where the second inequality holds because  $1/4 \leq 1/2 - \delta \leq f_{\mu}(t)$  with  $\delta \leq 1/4$ . Consider functions  $\tilde{f}_y^{(1)}, \dots, \tilde{f}_y^{(m)} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\tilde{f}_y^{(j)}(x, t) = f_{\text{mult}}^{(2)} \left( f_{\text{rec}}(f_{\mu}(t)), x + f_{\text{mult}}^{(2)} \left( f_y^{(j)}(x, t), f_{\sigma}(t) \right) \right), \quad j \in [m]$$

for  $x, t \in \mathbb{R}$ . Then, Lemma 9, Lemma 10, Lemma 11 and Lemma 12 imply that  $\tilde{f}_y^{(j)} \in \mathcal{F}_{\text{NN}}(\tilde{L}_x, \tilde{\mathbf{d}}_x, \tilde{s}_x, \tilde{M}_x^{(j)})$  for  $j \in [m]$  with

$$\begin{aligned} \tilde{L}_x &\leq D_7 \{\log(1/\delta)\}^2 \log \log(1/\delta), \quad \|\tilde{\mathbf{d}}_x\|_{\infty} \leq D_7 \{\log(1/\delta)\}^3, \\ \tilde{s}_x &\leq D_7 \{\log(1/\delta)\}^5 \log \log(1/\delta), \quad \tilde{M}_x^{(j)} \leq \exp \left( D_7 \{\log(1/\delta)\}^2 \right), \end{aligned} \quad (54)$$

where  $D_7 = D_7(C_{N,4}, C_{N,5}, D_3, D_6)$ . Note that both  $|\sigma_t|$  and  $|g_y^{(j)}(x, t)|$  are less than  $\{\log(1/\delta)\}^{\tau_{\text{mult}}}$  for  $|x| \leq 1$  and  $\delta \leq t \leq (2\bar{\tau})^{-1}$  with small enough  $\delta$ , due to the (27) and (51). Then,

$$\left| \sigma_t g_y^{(j)}(x, t) - f_{\text{mult}}^{(2)} \left( f_y^{(j)}(x, t), f_\sigma(t) \right) \right| \leq \delta + 2D_4 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + \frac{3}{2})\tau_{\text{mult}}}$$

for  $x \in [-1, 1]$  and  $\delta \leq t \leq (2\bar{\tau})^{-1}$ , where the inequality holds by combining (45) and (51) with (47). Also, both  $|x + \sigma_t g_y^{(j)}(x, t)|$  and  $|\mu_t^{-1}|$  are less than  $\{\log(1/\delta)\}^{\tau_{\text{mult}}}$  for  $|x| \leq 1$  and  $\delta \leq t \leq (2\bar{\tau})^{-1}$  with small enough  $\delta$ , due to the (27) and (51). Combining (53) and (47) with the last display, we have

$$\begin{aligned} & \left| \frac{x + \sigma_t g_y^{(j)}(x, t)}{\mu_t} - \tilde{f}_y^{(j)}(x, t) \right| \\ & \leq \delta + 2\{\log(1/\delta)\}^{\tau_{\text{mult}}} \max \left( 17\delta, \delta + 2D_4 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + \frac{3}{2})\tau_{\text{mult}}} \right) \\ & \leq D_8 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + \frac{5}{2})\tau_{\text{mult}}} \end{aligned} \quad (55)$$

for  $x \in [-1, 1]$  and  $\delta \leq t \leq (2\bar{\tau})^{-1}$ , where  $D_8 = 35 + 2D_4$ . Consider functions  $g_w^{(1)}, \dots, g_w^{(m)} : [0, \infty) \rightarrow \mathbb{R}$  and  $f_w^{(1)}, \dots, f_w^{(m)} : \mathbb{R} \rightarrow \mathbb{R}$  such that

$$g_w^{(j)}(t) = 2\sqrt{2\tau_{\text{tail}}} n_\beta \tilde{w}_{j - n_\beta \lfloor \frac{j}{n_\beta} \rfloor} \{\log(1/\sigma_t)\}^{\tau_{\text{bd}} + \frac{1}{2}}$$

for  $t \in [0, \infty)$  and

$$f_w^{(j)}(t) = 2\sqrt{2\tau_{\text{tail}}} n_\beta \tilde{w}_{j - n_\beta \lfloor \frac{j}{n_\beta} \rfloor} f_{\text{pow}}^{(\tau_{\text{bd}} + \frac{1}{2})} (f_{\log}(f_\sigma(t)))$$

for  $t \in \mathbb{R}$ . By (50), we have

$$\left| g_w^{(j)}(t) - f_w^{(j)}(t) \right| \leq D_9 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} - \frac{1}{2})\tau_{\text{mult}}}, \quad (56)$$

for  $\delta \leq t \leq (2\bar{\tau})^{-1}$ , where  $D_9 = 2\sqrt{2\tau_{\text{tail}}} D_2 n_\beta \max_{j \in [n_\beta]} \tilde{w}_j$ . Also, Lemma 9 and Lemma 10 implies that  $f_w^{(j)} \in \mathcal{F}_{\text{NN}}(L_w, \mathbf{d}_w, s_w, M_w^{(j)})$  for  $j \in [m]$  with

$$\begin{aligned} L_w & \leq L_{\text{mult}}^{(2)} + L_{\text{pl}\sigma} \vee L_\mu \leq D_{10} \{\log(1/\delta)\}^2 \log \log(1/\delta), \\ \|\mathbf{d}_w\|_\infty & \leq 4 \left\{ \|\mathbf{d}_{\text{mult}}^{(2)}\|_\infty \vee (\|\mathbf{d}_{\text{pl}\sigma}\|_\infty \vee \|\mathbf{d}_\mu\|_\infty) \right\} \leq D_{10} \{\log(1/\delta)\}^3, \\ s_w & \leq 4 \left\{ s_{\text{mult}}^{(2)} + 2(L_{\text{pl}\sigma} \vee L_\mu) + s_{\text{pl}\sigma} + s_\mu \right\} \leq D_{10} \{\log(1/\delta)\}^5 \log \log(1/\delta) \\ M_w^{(j)} & \leq \max \left\{ 2\sqrt{2\tau_{\text{tail}}} n_\beta \max_{j \in [n_\beta]} \tilde{w}_j, M_{\text{mult}}^{(2)}, M_{\text{pl}\sigma}, M_\mu, 1 \right\} \leq \exp(D_{10} \{\log(1/\delta)\}^2), \end{aligned} \quad (57)$$

where  $D_{10} = D_{10}(\beta, \tau_{\text{tail}}, C_{N,1}, C_{N,4}, D_5)$ . Consider a function  $\mathbf{f}_{\text{pre}} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{3mD}$  such that

$$\begin{aligned} (\mathbf{f}_{\text{pre}}(\mathbf{x}, t))_{3m(i-1)+3(j-1)+1} & = f_y^{(j)}(x_i, t), & (\mathbf{f}_{\text{pre}}(\mathbf{x}, t))_{3m(i-1)+3(j-1)+2} & = \tilde{f}_y^{(j)}(x_i, t), \\ (\mathbf{f}_{\text{pre}}(\mathbf{x}, t))_{3m(i-1)+3(j-1)+3} & = f_w^{(j)}(t), & i \in [D], j \in [m] \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . Combining Lemma 10 with (52), (54) and (57), we have  $\mathbf{f}_{\text{pre}} \in \mathcal{F}_{\text{NN}}(L_{\text{pre}}, \mathbf{d}_{\text{pre}}, s_{\text{pre}}, M_{\text{pre}})$  with

$$\begin{aligned} L_{\text{pre}} &\leq \max(L_x, \tilde{L}_x, L_w) \leq D_{11} \{\log(1/\delta)\}^2 \log \log(1/\delta), \\ \|\mathbf{d}_{\text{pre}}\|_\infty &\leq 2 \left( mD \|\mathbf{d}_x\|_\infty + mD \|\tilde{\mathbf{d}}_x\|_\infty + mD \|\mathbf{d}_w\|_\infty \right) \leq D_{11} m \{\log(1/\delta)\}^3, \\ s_{\text{pre}} &\leq 2 \left\{ 3mD \max(L_x, \tilde{L}_x, L_w) + mD s_x + mD \tilde{s}_x + mD s_w \right\} \\ &\leq D_{11} m \{\log(1/\delta)\}^5 \log \log(1/\delta), \\ M_{\text{pre}} &\leq \max(M_x, \tilde{M}_x, M_w, 1) \leq \exp(D_{11} \{\log(1/\delta)\}^2), \end{aligned}$$

where  $D_{11} = D_{11}(D, D_6, D_7, D_{10})$ .

The assumption **(S)** implies that  $p_0 = g_2 \circ \mathbf{g}_1$  for functions  $\mathbf{g}_1 : [-1, 1]^D \rightarrow [-K, K]^{|\mathcal{I}|}$  and  $g_2 : [-K, K]^{|\mathcal{I}|} \rightarrow \mathbb{R}$ , where  $\mathbf{g}_1 = (g_{11}, \dots, g_{1|\mathcal{I}|})$  with  $g_{1i} \in \mathcal{H}^{\beta, K}([-1, 1]^{|I|})$ ,  $I \in \mathcal{I}$  and  $g_2(x_1, \dots, x_{|\mathcal{I}|}) = \prod_{i=1}^{|\mathcal{I}|} x_i$  for  $x_1, \dots, x_{|\mathcal{I}|} \in [-K, K]$ . A simple calculation yields that  $g_2 \in \mathcal{H}^{\gamma, \tilde{K}}([-K, K]^{|\mathcal{I}|})$  with  $\tilde{K} = (2K)^{|\mathcal{I}|}$  for any  $\gamma \geq |\mathcal{I}| + 1$ . Since  $|\mathcal{I}| \leq 2^D$ , Lemma 5 of Chae et al. (2023) implies that there exists neural networks  $f_{p_0} \in \mathcal{F}_{\text{NN}}(L_{p_0}, \mathbf{d}_{p_0}, s_{p_0}, M_{p_0})$  with

$$L_{p_0} \leq D_{12} \log m, \quad \|\mathbf{d}_{p_0}\|_\infty \leq D_{12} m, \quad s_{p_0} \leq D_{12} m \log m, \quad M_{p_0} \leq 1$$

such that  $|p_0(\mathbf{x}) - f_{p_0}(\mathbf{x})| \leq m^{-\frac{\beta}{d}}$  for  $\|\mathbf{x}\|_\infty \leq 1$ , where  $D_{12} = D_{12}(\beta, d, D, K)$ . Since  $p_0 \in \mathcal{H}^{\beta, K}([-1, 1]^D)$ , we have  $|p_0(\mathbf{x}) - p_0(\tilde{\mathbf{x}})| \leq KD \|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty^{\beta \wedge 1}$  for any  $\mathbf{x}, \tilde{\mathbf{x}} \in [-1, 1]^D$ . Let  $\tilde{C}_2$  be the constant in Lemma 22. Then, we have

$$\left| \frac{x + \sigma_t g_y^{(j)}(x, t)}{\mu_t} \right| \leq 1 - \frac{\{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}}{2} < 1$$

for  $|x| \leq \mu_t - \mu_t \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $\delta \leq t \leq \bar{\tau}^{-1}(\tilde{C}_2^2 \wedge 1/4)$ . Combining with (55), we have

$$\begin{aligned} &\left| p_0 \left( \frac{\mathbf{x} + \sigma_t \left( g_y^{(j_1)}(x_1, t), \dots, g_y^{(j_D)}(x_D, t) \right)^\top}{\mu_t} \right) - f_{p_0} \left( \tilde{f}_y^{(j_1)}(x_1, t), \dots, \tilde{f}_y^{(j_D)}(x_D, t) \right) \right| \quad (58) \\ &\leq K D D_8^{\beta \wedge 1} \delta^{\frac{\beta \wedge 1}{2}} \{\log(1/\delta)\}^{(\beta \wedge 1)(\tau_{\text{bd}} + \frac{5}{2}) \tau_{\text{mult}}} + m^{-\frac{\beta}{d}} \stackrel{\text{def}}{=} \epsilon_{p_0}, \quad j_1, \dots, j_D \in [m] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t - \mu_t \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $\delta \leq t \leq \bar{\tau}^{-1}(\tilde{C}_2^2 \wedge 1/4)$ . Let  $C_{N,3}$  be the constant in Lemma 17. Then, there exists a neural network  $f_{\text{exp}} \in \mathcal{F}_{\text{NN}}(L_{\text{exp}}, \mathbf{d}_{\text{exp}}, s_{\text{exp}}, M_{\text{exp}})$  with

$$\begin{aligned} L_{\text{exp}} &\leq C_{N,3} \log(1/\delta) \log \log(1/\delta), \quad \|\mathbf{d}_{\text{exp}}\|_\infty \leq C_{N,3} \{\log(1/\delta)\}^3, \\ s_{\text{exp}} &\leq C_{N,3} \{\log(1/\delta)\}^4, \quad M_{\text{exp}} \leq C_{N,3} \delta^{-1}, \end{aligned}$$

such that  $|e^{-x} - f_{\text{exp}}(\tilde{x})| \leq \delta + |x - \tilde{x}|$  for any  $x \geq 0$  and  $\tilde{x} \in \mathbb{R}$ . Consider a function  $f_\phi : \mathbb{R}^D \rightarrow \mathbb{R}$  such that

$$f_\phi(\mathbf{x}) = (2\pi)^{-\frac{D}{2}} f_{\text{exp}} \left( \sum_{i=1}^D \frac{f_{\text{pow}}^{(2)}(x_i)}{2} \right)$$

for  $\mathbf{x} = (x_1, \dots, x_D) \in \mathbb{R}^D$ . Then, Lemma 9, Lemma 10 and Lemma 11 imply that  $f_\phi \in \mathcal{F}_{\text{NN}}(L_\phi, \mathbf{d}_\phi, s_\phi, M_\phi)$  with

$$\begin{aligned} L_\phi &\leq D_{13} \log(1/\delta) \log \log(1/\delta), \quad \|\mathbf{d}_\phi\|_\infty \leq D_{13} \{\log(1/\delta)\}^3 \\ s_\phi &\leq D_{13} \{\log(1/\delta)\}^4, \quad M_\phi \leq D_{13} \delta^{-1}, \end{aligned}$$

where  $D_{13} = D_{13}(D, C_{N,1}, C_{N,3})$ . Combining (51) with (48), it follows that

$$\begin{aligned} &\left| \prod_{i=1}^D \phi \left( g_y^{(j_i)}(x_i, t) \right) - f_\phi \left( f_y^{(j_1)}(x_1, t), \dots, f_y^{(j_D)}(x_D, t) \right) \right| \\ &\leq (2\pi)^{-\frac{D}{2}} \left[ \delta + \left| \sum_{i=1}^D \frac{\left\{ g_y^{(j_i)}(x_i, t) \right\}^2 - f_{\text{pow}}^{(2)} \left( f_y^{(j_i)}(x_i, t) \right)}{2} \right| \right] \\ &\leq (2\pi)^{-\frac{D}{2}} \left[ \delta + \frac{1}{2} \sum_{i=1}^D \left( \delta + 2 \{\log(1/\delta)\}^{\tau_{\text{mult}}} \left| g_y^{(j_i)}(x_i, t) - f_y^{(j_i)}(x_i, t) \right| \right) \right] \\ &\leq D_{14} \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + \frac{3}{2})\tau_{\text{mult}}} \stackrel{\text{def}}{=} \epsilon_\phi, \quad j_1, \dots, j_D \in [m] \end{aligned} \tag{59}$$

for  $\|\mathbf{x}\|_\infty \leq 1$  and  $\delta \leq t \leq (2\bar{\tau})^{-1}$ , where  $D_{14} = D_{14}(D, D_4)$ . Combining (56) with (47), we have

$$\begin{aligned} &\left| \prod_{i=1}^D g_w^{(j_i)}(t) - f_{\text{mult}}^{(D)} \left( f_w^{(j_1)}(t), \dots, f_w^{(j_D)}(t) \right) \right| \\ &\leq \delta + DD_9 \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + D - \frac{3}{2})\tau_{\text{mult}}} \\ &\leq D_{15} \sqrt{\delta} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + D - \frac{3}{2})\tau_{\text{mult}}} \stackrel{\text{def}}{=} \epsilon_w \end{aligned} \tag{60}$$

for  $\delta \leq t \leq (2\bar{\tau})^{-1}$  with small enough  $\delta$  so that  $|g_w^{(j_i)}(t)| \leq \{\log(1/\delta)\}^{\tau_{\text{bd}}}$  for each  $j_i \in [m]$ , where  $D_{15} = 1 + DD_9$ .

Note that  $|p_0(\mathbf{x})| \leq K$  for any  $\|\mathbf{x}\|_\infty \leq 1$ ,  $|\phi(x)| \leq 1/\sqrt{2\pi}$  for any  $x \in \mathbb{R}$  and  $|g_y^{(j)}(\mathbf{x}, t)|, |g_w^{(j)}(t)| \leq D_{16} \{\log(1/\delta)\}^{\tau_{\text{bd}} + \frac{1}{2}}$  for  $j \in [m]$ ,  $\|\mathbf{x}\|_\infty \leq 1, \delta \leq t \leq (4\bar{\tau})^{-1}$ , where  $D_{16} = 2\sqrt{2\tau_{\text{tail}}}(2 + n_\beta) \max_{j \in [n_\beta]} \tilde{w}_j$ . Let  $\tilde{f}_{\text{mult}}^{(2)} \in \mathcal{F}_{\text{NN}}(\tilde{L}_{\text{mult}}^{(2)}, \tilde{\mathbf{d}}_{\text{mult}}^{(2)}, \tilde{s}_{\text{mult}}^{(2)}, \tilde{M}_{\text{mult}}^{(2)})$  be the neural network in Lemma 14, with

$$\begin{aligned} \tilde{L}_{\text{mult}}^{(2)} &\leq C_{N,1} \log 2 \{ (2D\tau_{\text{bd}} + D + 2) \log(1/\delta) + D \log D_{16} \}, \\ \|\tilde{\mathbf{d}}_{\text{mult}}^{(2)}\|_\infty &\leq 96, \\ \tilde{s}_{\text{mult}}^{(2)} &\leq 2C_{N,1} \{ (D\tau_{\text{bd}} + D/2 + 1) \log(1/\delta) + D \log D_{16} \}, \\ \tilde{M}_{\text{mult}}^{(2)} &= D_{16}^{2D} \{\log(1/\delta)\}^{2D(\tau_{\text{bd}} + \frac{1}{2})} \end{aligned}$$

such that

$$|\tilde{f}_{\text{mult}}^{(2)}(\tilde{\mathbf{x}}) - x_1 x_2| \leq \delta + 2D_{16}^D \{\log(1/\delta)\}^{D(\tau_{\text{bd}} + \frac{1}{2})} \tilde{\epsilon}$$

for all  $\|\mathbf{x}\|_\infty \leq D_{16}^D \{\log(1/\delta)\}^{D(\tau_{\text{bd}} + \frac{1}{2})}$ ,  $\tilde{\mathbf{x}} \in \mathbb{R}^2$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ . Also, let

$$\bar{f}_{\text{mult}}^{(3)} \in \mathcal{F}_{\text{NN}}(\bar{L}_{\text{mult}}^{(3)}, \bar{\mathbf{d}}_{\text{mult}}^{(3)}, \bar{s}_{\text{mult}}^{(3)}, \bar{M}_{\text{mult}}^{(3)})$$

be the neural network in Lemma 14 with

$$\begin{aligned} \bar{L}_{\text{mult}}^{(3)} &\leq C_{N,1} \log 3 \{\log(1/\delta) + 3 \log(K \vee 1)\}, & \|\bar{\mathbf{d}}_{\text{mult}}^{(3)}\|_\infty &\leq 144, \\ \bar{s}_{\text{mult}}^{(3)} &\leq 3C_{N,1} \{\log(1/\delta) + \log(K \vee 1)\}, & \bar{M}_{\text{mult}}^{(3)} &= K^3 \vee 1 \end{aligned}$$

such that

$$|\bar{f}_{\text{mult}}^{(3)}(\tilde{\mathbf{x}}) - x_1 x_2 x_3| \leq \delta + 3(K^2 \vee 1)\tilde{\epsilon}$$

for all  $\|\mathbf{x}\|_\infty \leq K \vee 1$ ,  $\tilde{\mathbf{x}} \in \mathbb{R}^3$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ . Consider functions  $\mathbf{f}_{\text{main}} : \mathbb{R}^D \times \mathbb{R}^D \times \mathbb{R}^D \rightarrow \mathbb{R}^{D+1}$  such that

$$\begin{aligned} (\mathbf{f}_{\text{main}}(\mathbf{x}, \tilde{\mathbf{x}}, \mathbf{w}))_i &= \tilde{f}_{\text{mult}}^{(2)} \left( \bar{f}_{\text{mult}}^{(3)}(x_i, f_{p_0}(\tilde{\mathbf{x}}), f_\phi(\mathbf{x})), f_{\text{mult}}^{(D)}(\mathbf{w}) \right), \quad i \in [D], \\ (\mathbf{f}_{\text{main}}(\mathbf{x}, \tilde{\mathbf{x}}, \mathbf{w}))_{D+1} &= \tilde{f}_{\text{mult}}^{(2)} \left( \bar{f}_{\text{mult}}^{(3)}(1, f_{p_0}(\tilde{\mathbf{x}}), f_\phi(\mathbf{x})), f_{\text{mult}}^{(D)}(\mathbf{w}) \right) \end{aligned}$$

for  $\mathbf{x} = (x_1, \dots, x_D) \in \mathbb{R}^D$  and  $\tilde{\mathbf{x}}, \mathbf{w} \in \mathbb{R}^D$ . Lemma 9, Lemma 10 and Lemma 12 implies that  $\mathbf{f}_{\text{main}} \in \mathcal{F}_{\text{NN}}(L_{\text{main}}, \mathbf{d}_{\text{main}}, s_{\text{main}}, M_{\text{main}})$  with

$$\begin{aligned} L_{\text{main}} &\leq D_{17} [\log m + \log(1/\delta) \log \log(1/\delta)], & \|\mathbf{d}_{\text{main}}\|_\infty &\leq D_{17} [m + \{\log(1/\delta)\}^3] \\ s_{\text{main}} &\leq D_{17} [m \log m + \{\log(1/\delta)\}^4], & M_{\text{main}} &\leq D_{17} \delta^{-1}, \end{aligned}$$

where  $D_{17} = D_{17}(D, K, C_{N,1}, D_{10}, D_{12}, D_{13}, D_{16})$ . For  $\mathbf{j} = (j_1, \dots, j_D) \in [m]^D$ , consider a function  $\mathbf{f}^{(\mathbf{j})} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{3D}$  such that

$$\begin{aligned} \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) &= \left( f_y^{(j_1)}(x_1, t), \dots, f_y^{(j_D)}(x_D, t), \tilde{f}_y^{(j_1)}(x_1, t), \dots, \tilde{f}_y^{(j_D)}(x_D, t), f_w^{(j_1)}(t), \dots, f_w^{(j_D)}(t) \right)^\top. \end{aligned}$$

By (58), (59) and (60), we have

$$\begin{aligned} &\left| p_0 \left( \frac{\mathbf{x} + \sigma_t \left( g_y^{(j_1)}(x_1, t), \dots, g_y^{(j_D)}(x_D, t) \right)^\top}{\mu_t} \right) \prod_{i=1}^D \phi \left( g_y^{(j_i)}(x_i, t) \right) g_w^{(j_i)}(t) \right. \\ &\quad \left. - \left( \mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) \right)_{D+1} \right| \\ &\leq \delta + 2D_{16}^D \{\log(1/\delta)\}^{D(\tau_{\text{bd}} + \frac{1}{2})} \max \{ \delta + 3(K^2 \vee 1) (\epsilon_{p_0} \vee \epsilon_\phi), \epsilon_w \} \\ &\leq D_{18} \{\log(1/\delta)\}^{D(\tau_{\text{bd}} + \frac{1}{2})} \left[ m^{-\frac{\beta}{d}} + \delta^{\frac{\beta \wedge 1}{2}} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + D + \frac{3}{2})\tau_{\text{mult}}} \right] \end{aligned}$$

and

$$\begin{aligned}
 & \left| g_y^{(j_k)}(x_k, t) p_0 \left( \frac{\mathbf{x} + \sigma_t \left( g_y^{(j_1)}(x_1, t), \dots, g_y^{(j_D)}(x_D, t) \right)^\top}{\mu_t} \right) \prod_{i=1}^D \phi \left( g_y^{(j_i)}(x_i, t) \right) g_w^{(j_i)}(t) \right. \\
 & \quad \left. - \left( \mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) \right)_k \right| \\
 & \leq \delta + 2D_{16}^D \{\log(1/\delta)\}^{D(\tau_{\text{bd}} + \frac{1}{2})} \max \{ \delta + 3(K^2 \vee 1) (\epsilon_{p_0} \vee \epsilon_\phi), \epsilon_w \} \\
 & \leq D_{18} \{\log(1/\delta)\}^{D(\tau_{\text{bd}} + \frac{1}{2})} \left[ m^{-\frac{\beta}{d}} + \delta^{\frac{\beta \wedge 1}{2}} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + D + \frac{3}{2})\tau_{\text{mult}}} \right], \quad k \in [D], j_1, \dots, j_D \in [m]
 \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t - \mu_t \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $\delta \leq t \leq \bar{\tau}^{-1}(\tilde{C}_2^2 \wedge 1/4)$ , where

$$D_{18} = D_{18}(\beta, D, K, D_8, D_{14}, D_{15}, D_{16}).$$

Let  $\tilde{C}_1$  be the constant in Lemma 22. It follows that

$$\begin{aligned}
 & \mu_t^D \left\| \frac{1}{m^D} \sum_{\mathbf{j} \in [m]^D} \mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) - \begin{pmatrix} \sigma_t \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} \right\|_\infty \\
 & \leq \tilde{C}_1 K \{\log(1/\sigma_t)\}^{(\tau_{\text{bd}} + \frac{1}{2})(D-1)} \left( \sigma_t^{\tau_{\text{tail}}} + m^{-\beta} \{\log(1/\sigma_t)\}^{(\tau_{\text{bd}} + \frac{1}{2})(\beta+1)} \right) \\
 & \quad + D_{18} \{\log(1/\delta)\}^{D(\tau_{\text{bd}} + \frac{1}{2})} \left[ m^{-\frac{\beta}{d}} + \delta^{\frac{\beta \wedge 1}{2}} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + D + \frac{3}{2})\tau_{\text{mult}}} \right]
 \end{aligned}$$

for  $\delta \leq t \leq \bar{\tau}^{-1}(\tilde{C}_2^2 \wedge 1/2)$ . Let

$$m = n_\beta \lfloor \tilde{m} \rfloor \quad \text{and} \quad \delta = \tilde{m}^{-\tau_{\text{min}}}$$

with large enough  $\tilde{m} > 0$ . Since  $\tau_{\text{min}} \geq \frac{4\beta}{d(\beta \wedge 1)}$ , we have  $\delta^{\frac{\beta \wedge 1}{2}} \{\log(1/\delta)\}^{(\tau_{\text{bd}} + D + \frac{3}{2})\tau_{\text{mult}}} \leq \tilde{m}^{-\frac{\beta}{d}}$  for large enough  $\tilde{m}$ . Then,

$$\begin{aligned}
 & \left\| \frac{1}{m^D} \sum_{\mathbf{j} \in [m]^D} \mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) - \begin{pmatrix} \sigma_t \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} \right\|_\infty \\
 & \leq D_{19} (\log \tilde{m})^{(\tau_{\text{bd}} + \frac{1}{2})(D-1)} \left\{ t^{\frac{\tau_{\text{tail}}}{2}} + \tilde{m}^{-\frac{\beta}{d}} (\log \tilde{m})^{(\tau_{\text{bd}} + \frac{1}{2})(\beta+1)} \right\}, \tag{61}
 \end{aligned}$$

where  $D_{19} = D_{19}(\beta, K, D, d, \tau_{\text{bd}}, \tau_{\text{tail}}, \tau_{\text{min}}, \bar{\tau}, \underline{\tau}, \tilde{C}_1, D_{18})$ .

Recall that  $\mathbf{f}_{\text{pre}} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{3mD}$  and  $\mathbf{f}_{\text{main}} : \mathbb{R}^{3D} \rightarrow \mathbb{R}^{D+1}$ . Define a function  $\tilde{\mathbf{f}}_{\text{pre}} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{6mD}$  as

$$\tilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) = \rho \begin{pmatrix} \mathbf{f}_{\text{pre}}(\mathbf{x}, t) \\ -\mathbf{f}_{\text{pre}}(\mathbf{x}, t) \end{pmatrix}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . For each  $\mathbf{j} = (j_1, \dots, j_D) \in [m]^D$ , there exists a  $6mD \times 6mD$  permutation matrix  $Q_1^{(\mathbf{j})}$  such that

$$Q_1^{(\mathbf{j})} \tilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) = \rho \begin{pmatrix} \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \\ -\mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \\ \mathbf{0}_{6mD-6D} \end{pmatrix} \in \mathbb{R}^{6mD}.$$

Let  $W_1, \mathbf{b}_1, \dots, W_{L_{\text{main}}}, \mathbf{b}_{L_{\text{main}}}$  be the weight matrices and shift vectors of the neural network  $\mathbf{f}_{\text{main}}$ , where  $\mathbf{d}_{\text{main}} = (d_1, \dots, d_{L_{\text{main}}+1})$  with  $d_1 = 3D$ ,  $d_{L_{\text{main}}+1} = D + 1$  and  $W_l \in \mathbb{R}^{d_{l+1} \times d_l}$ ,  $\mathbf{b}_l \in \mathbb{R}^{d_{l+1}}$  for  $l \in [L_{\text{main}}]$ . Since  $x \vee 0 - (-x \vee 0) = x$  for any  $x \in \mathbb{R}$ , we have

$$\widetilde{W}_1 Q_1^{(\mathbf{j})} \widetilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) + \widetilde{\mathbf{b}}_1 = \begin{pmatrix} W_1 \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) + \mathbf{b}_1 \\ \mathbf{0}_{m^D d_2 - d_2} \end{pmatrix} \in \mathbb{R}^{m^D d_2}, \quad \forall \mathbf{j} \in [m]^D,$$

where

$$\widetilde{W}_1 = \begin{pmatrix} W_1 & -W_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{m^D d_2 \times 6mD}, \quad \widetilde{\mathbf{b}}_1 = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{0} \end{pmatrix} \in \mathbb{R}^{m^D d_2}.$$

For each  $\mathbf{j} \in [m]^D$ , there exists a  $m^D d_2 \times m^D d_2$  permutation matrix  $R_1^{(\mathbf{j})}$  such that

$$R_1^{(\mathbf{j})} \left( \widetilde{W}_1 Q_1^{(\mathbf{j})} \widetilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) + \widetilde{\mathbf{b}}_1 \right) = \begin{pmatrix} \mathbf{0}_{d_2 \sum_{i=1}^D m^{i-1}(j_i-1)} \\ W_1 \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) + \mathbf{b}_1 \\ \mathbf{0}_{m^D d_2 - d_2 \sum_{i=1}^D m^{i-1}(j_i-1) - d_2} \end{pmatrix} \in \mathbb{R}^{m^D d_2}.$$

It follows that

$$\begin{aligned} & \left( \sum_{\mathbf{j} \in [m]^D} R_1^{(\mathbf{j})} \left( \widetilde{W}_1 Q_1^{(\mathbf{j})} \widetilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) + \widetilde{\mathbf{b}}_1 \right) \right)_{d_2 \sum_{i=1}^D m^{i-1}(\tilde{j}_i-1)+1: d_2 \sum_{i=1}^D m^{i-1}(\tilde{j}_i-1)+d_2} \\ &= W_1 \mathbf{f}^{(\tilde{\mathbf{j}})}(\mathbf{x}, t) + \mathbf{b}_1, \quad \forall \tilde{\mathbf{j}} = (\tilde{j}_1, \dots, \tilde{j}_D) \in [m]^D. \end{aligned}$$

Let  $\tilde{\mathbf{d}} = (\tilde{d}_1, \dots, \tilde{d}_{L_{\text{main}}+2})$ , where  $\tilde{d}_1 = 2md_1 = 6mD$ ,  $\tilde{d}_l = m^D d_l$ ,  $l \in \{2, \dots, L_{\text{main}}\}$ ,  $\tilde{d}_{L_{\text{main}}+1} = 2m^D d_{L_{\text{main}}+1} = 2m^D(D+1)$  and  $\tilde{d}_{L_{\text{main}}+2} = 2d_{L_{\text{main}}+1} = 2(D+1)$ . For each  $l \in \{2, \dots, L_{\text{main}} - 1\}$ , define block-sparse matrix and vector as

$$\widetilde{W}_l = \begin{pmatrix} W_l & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{\tilde{d}_{l+1} \times \tilde{d}_l} \quad \text{and} \quad \widetilde{\mathbf{b}}_l = \begin{pmatrix} \mathbf{b}_l \\ \mathbf{0} \end{pmatrix} \in \mathbb{R}^{\tilde{d}_{l+1}}.$$

Moreover, for each  $l \in \{2, \dots, L_{\text{main}} - 1\}$  and  $\mathbf{j} \in [m]^D$ , there exist  $\tilde{d}_l \times \tilde{d}_l$  permutation matrix  $Q_l^{(\mathbf{j})}$  and  $\tilde{d}_{l+1} \times \tilde{d}_{l+1}$  permutation matrix  $R_l^{(\mathbf{j})}$  such that

$$R_l^{(\mathbf{j})} \left( \widetilde{W}_l Q_l^{(\mathbf{j})} \mathbf{z} + \widetilde{\mathbf{b}}_l \right) = \rho \left( \begin{pmatrix} \mathbf{0}_{d_{l+1} \sum_{i=1}^D m^{i-1}(j_i-1)} \\ W_l \mathbf{z}_{d_l \sum_{i=1}^D m^{i-1}(j_i-1)+1: d_l \sum_{i=1}^D m^{i-1}(j_i-1)+d_l} + \mathbf{b}_l \\ \mathbf{0}_{m^D d_{l+1} - d_{l+1} \sum_{i=1}^D m^{i-1}(j_i-1) - d_{l+1}} \end{pmatrix} \right), \quad \mathbf{z} \in \mathbb{R}^{\tilde{d}_l},$$

where  $\mathbf{z}_{n_1:n_2} \in \mathbb{R}^{n_2-n_1+1}$  denotes the subvector of  $\mathbf{z}$  from  $n_1$ -th component to  $n_2$ -th component. It follows that

$$\begin{aligned} & \left( \widetilde{\mathbf{f}}_{L_{\text{main}}-1} \circ \dots \circ \widetilde{\mathbf{f}}_1 \circ \widetilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) \right)_{d_{L_{\text{main}}} \sum_{i=1}^D m^{i-1}(j_i-1)+1: d_{L_{\text{main}}} \sum_{i=1}^D m^{i-1}(j_i-1)+d_{L_{\text{main}}}} \\ &= \rho(W_{L_{\text{main}}-1} \cdot + \mathbf{b}_{L_{\text{main}}-1}) \circ \dots \circ \rho(W_1 \cdot + \mathbf{b}_1) \circ \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t), \quad \forall \mathbf{j} \in [m]^D, \end{aligned}$$

where  $\tilde{\mathbf{f}}_l : \mathbb{R}^{\tilde{d}_l} \rightarrow \mathbb{R}^{\tilde{d}_{l+1}}$  is a vector-valued function defined as

$$\tilde{\mathbf{f}}_l(\mathbf{z}) = \rho \left( \sum_{\mathbf{j} \in [m]^D} R_l^{(\mathbf{j})} \left( \tilde{W}_l Q_l^{(\mathbf{j})} \mathbf{z} + \tilde{\mathbf{b}}_l \right) \right), \quad l \in [L_{\text{main}} - 1].$$

Let  $\tilde{W}_{L_{\text{main}}}$  and  $\tilde{\mathbf{b}}_{L_{\text{main}}}$  be the block-sparse matrix and vector, respectively, defined as

$$\tilde{W}_{L_{\text{main}}} = \begin{pmatrix} W_{L_{\text{main}}} & \mathbf{0} \\ -W_{L_{\text{main}}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{\tilde{d}_{L_{\text{main}}+1} \times \tilde{d}_{L_{\text{main}}}} \quad \text{and} \quad \tilde{\mathbf{b}}_{L_{\text{main}}} = \begin{pmatrix} \mathbf{b}_{L_{\text{main}}} \\ -\mathbf{b}_{L_{\text{main}}} \\ \mathbf{0} \end{pmatrix} \in \mathbb{R}^{\tilde{d}_{L_{\text{main}}+1}}.$$

For each  $\mathbf{j} \in [m]^D$ , there exist  $\tilde{d}_{L_{\text{main}}} \times \tilde{d}_{L_{\text{main}}}$  permutation matrix  $Q_{L_{\text{main}}}^{(\mathbf{j})}$  and  $\tilde{d}_{L_{\text{main}}+1} \times \tilde{d}_{L_{\text{main}}+1}$  permutation matrix  $R_{L_{\text{main}}}^{(\mathbf{j})}$  such that

$$\begin{aligned} & \left( \tilde{\mathbf{f}}_{L_{\text{main}}} \circ \cdots \circ \tilde{\mathbf{f}}_1 \circ \tilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) \right)_{2d_{L_{\text{main}}+1} \sum_{i=1}^D m^{i-1}(j_i-1)+1:2d_{L_{\text{main}}+1} \sum_{i=1}^D m^{i-1}(j_i-1)+d_{L_{\text{main}}+1}} \\ &= \rho(W_{L_{\text{main}}} \cdot + \mathbf{b}_{L_{\text{main}}}) \circ \rho(W_{L_{\text{main}}-1} \cdot + \mathbf{b}_{L_{\text{main}}-1}) \circ \cdots \circ \rho(W_1 \cdot + \mathbf{b}_1) \circ \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \\ &= \rho \left( \mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) \right) \end{aligned}$$

and

$$\begin{aligned} & \left( \tilde{\mathbf{f}}_{L_{\text{main}}} \circ \cdots \circ \tilde{\mathbf{f}}_1 \circ \tilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) \right)_{2d_{L_{\text{main}}+1} \sum_{i=1}^D m^{i-1}(j_i-1)+d_{L_{\text{main}}+1}+1:2d_{L_{\text{main}}+1} \sum_{i=1}^D m^{i-1}(j_i-1)+2d_{L_{\text{main}}+1}} \\ &= \rho(-W_{L_{\text{main}}} \cdot - \mathbf{b}_{L_{\text{main}}}) \circ \rho(W_{L_{\text{main}}-1} \cdot + \mathbf{b}_{L_{\text{main}}-1}) \circ \cdots \circ \rho(W_1 \cdot + \mathbf{b}_1) \circ \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \\ &= \rho \left( -\mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) \right), \end{aligned}$$

where  $\tilde{\mathbf{f}}_{L_{\text{main}}} : \mathbb{R}^{\tilde{d}_{L_{\text{main}}}} \rightarrow \mathbb{R}^{\tilde{d}_{L_{\text{main}}+1}}$  is a vector-valued function defined as

$$\tilde{\mathbf{f}}_{L_{\text{main}}}(\mathbf{z}) = \rho \left( \sum_{\mathbf{j} \in [m]^D} R_{L_{\text{main}}}^{(\mathbf{j})} \left( \tilde{W}_{L_{\text{main}}} Q_{L_{\text{main}}}^{(\mathbf{j})} \mathbf{z} + \tilde{\mathbf{b}}_{L_{\text{main}}} \right) \right).$$

Let  $\tilde{W}_{L_{\text{main}}+1}$  be a block-sparse matrix, defined as

$$\tilde{W}_{L_{\text{main}}+1} = \begin{pmatrix} m^{-D} \mathbb{I}_{D+1} & -m^{-D} \mathbb{I}_{D+1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{\tilde{d}_{L_{\text{main}}+2} \times \tilde{d}_{L_{\text{main}}+1}}.$$

For each  $\mathbf{j} \in [m]^D$ , there exist  $\tilde{d}_{L_{\text{main}}+1} \times \tilde{d}_{L_{\text{main}}+1}$  permutation matrix  $Q_{L_{\text{main}}+1}^{(\mathbf{j})}$  and  $\tilde{d}_{L_{\text{main}}+2} \times \tilde{d}_{L_{\text{main}}+2}$  permutation matrix  $R_{L_{\text{main}}+1}^{(\mathbf{j})}$  such that

$$(\mathbf{f}_1(\mathbf{x}, t))_{1:D+1} = \rho \left( m^{-D} \sum_{\mathbf{j} \in [m]^D} \mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) \right)$$

and

$$(\mathbf{f}_1(\mathbf{x}, t))_{D+2:2D+2} = \rho \left( -m^{-D} \sum_{\mathbf{j} \in [m]^D} \mathbf{f}_{\text{main}} \left( \mathbf{f}^{(\mathbf{j})}(\mathbf{x}, t) \right) \right),$$

where

$$\mathbf{f}_1(\mathbf{x}, t) = \rho \left( \sum_{\mathbf{j} \in [m]^D} R_{L_{\text{main}}+1}^{(\mathbf{j})} \widetilde{W}_{L_{\text{main}}+1} Q_{L_{\text{main}}+1}^{(\mathbf{j})} \widetilde{\mathbf{f}}_{L_{\text{main}}} \circ \cdots \circ \widetilde{\mathbf{f}}_1 \circ \widetilde{\mathbf{f}}_{\text{pre}}(\mathbf{x}, t) \right).$$

Combining with (61), we have

$$\begin{aligned} & \left\| \mathbf{f}(\mathbf{x}, t) - \begin{pmatrix} \sigma_t \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} \right\|_{\infty} \\ & \leq D_{19} (\log \tilde{m})^{(\tau_{\text{bd}} + \frac{1}{2})(D-1)} \left\{ t^{\frac{\tau_{\text{tail}}}{2}} + \tilde{m}^{-\frac{\beta}{d}} (\log \tilde{m})^{(\tau_{\text{bd}} + \frac{1}{2})(\beta+1)} \right\} \end{aligned} \quad (62)$$

for  $\|\mathbf{x}\|_{\infty} \leq \mu_t - \mu_t \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $\tilde{m}^{-\tau_{\text{min}}} \leq t \leq \bar{\tau}^{-1}(\tilde{C}_2^2 \wedge 1/2)$ , where  $\mathbf{f} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{D+1}$  is a vector-valued function, defined as

$$\mathbf{f}(\mathbf{x}, t) = (\mathbb{I}_{D+1} \quad -\mathbb{I}_{D+1}) \mathbf{f}_1(\mathbf{x}, t).$$

Note that  $\|\widetilde{W}_l\|_0 = \|W_l\|_0$ ,  $\|\widetilde{\mathbf{b}}_l\|_0 = \|\mathbf{b}_l\|_0$  for  $l \in \{2, \dots, L_{\text{main}} - 1\}$ ,  $\|\widetilde{W}_1\|_0 = 2\|W_1\|_0$ ,  $\|\widetilde{\mathbf{b}}_1\|_0 = 2\|\mathbf{b}_1\|_0$ ,  $\|\widetilde{W}_{L_{\text{main}}}\|_0 = 2\|W_{L_{\text{main}}}\|_0$ ,  $\|\widetilde{\mathbf{b}}_{L_{\text{main}}}\|_0 = 2\|\mathbf{b}_{L_{\text{main}}}\|_0$  and  $\|\widetilde{W}_{L_{\text{main}}+1}\|_0 = 2D$ . Let  $\bar{L} = L_{\text{pre}} + L_{\text{main}} + 2$  and  $\bar{\mathbf{d}} = (\bar{d}_1, \dots, \bar{d}_{\bar{L}+1}) \in \mathbb{N}^{\bar{L}+1}$  with

$$(\bar{d}_1, \dots, \bar{d}_{\bar{L}+1}) = (d_{\text{pre}}^{(1)}, \dots, d_{\text{pre}}^{(L_{\text{pre}})}, \tilde{d}_1, \dots, \tilde{d}_{L_{\text{main}}+2}, d_{L_{\text{main}}+1}),$$

where  $\mathbf{d}_{\text{pre}} = (d_{\text{pre}}^{(1)}, \dots, d_{\text{pre}}^{(L_{\text{pre}}+1)})$ . For  $1 \leq i \leq L_{\text{pre}}$ , let  $\mathcal{Q}_i$  and  $\mathcal{R}_i$  be the set of  $\bar{d}_i \times \bar{d}_i$  and  $\bar{d}_{i+1} \times \bar{d}_{i+1}$  identity matrix, respectively. For  $L_{\text{pre}} < i \leq L - 1$ , let

$$\mathcal{Q}_i = \left( Q_{i-L_{\text{pre}}}^{(\mathbf{j})} \right)_{\mathbf{j} \in [m]^D} \quad \text{and} \quad \mathcal{R}_i = \left( R_{i-L_{\text{pre}}}^{(\mathbf{j})} \right)_{\mathbf{j} \in [m]^D}.$$

Let  $\mathbf{m} = (m_1, \dots, m_{\bar{L}-1})$  with  $m_i = 1$  for  $i \leq L_{\text{pre}}$  and  $m_i = m^D$  for  $i > L_{\text{pre}}$ , and  $\mathcal{P} = ((\mathcal{Q}_i, \mathcal{R}_i))_{i \in [\bar{L}-1]}$ . Then,  $\mathbf{f} \in \mathcal{F}_{\text{WSNN}}(\bar{L}, \bar{\mathbf{d}}, \bar{s}, \bar{M}, \mathcal{P}_{\mathbf{m}})$  with

$$\bar{s} \leq 2s_{\text{pre}} + 2s_{\text{main}} + 4d_{L_{\text{main}}+1} \quad \text{and} \quad \bar{M} = \max(M_{\text{pre}}, M_{\text{main}}, 1, m^{-D}).$$

Recall that  $m = n_{\beta} \lfloor \tilde{m} \rfloor$  and  $\delta = \tilde{m}^{-\tau_{\text{min}}}$ . Thus,

$$\begin{aligned} \bar{L} & \leq D_{20} (\log \tilde{m})^2 \log \log \tilde{m}, \quad \|\bar{\mathbf{d}}\|_{\infty} \leq D_{20} \tilde{m}^{D+1}, \\ \bar{s} & \leq D_{20} \tilde{m} (\log \tilde{m})^5 \log \log \tilde{m}^{D+1}, \quad \bar{M} \leq \exp(D_{20} \{\log \tilde{m}\}^2), \end{aligned}$$

where  $D_{20} = D_{20}(\tau_{\text{min}}, D_{11}, D_{17}, n_{\beta})$ . Combining (62) with the last display, the assertion follows by re-defining the constants.  $\blacksquare$

### B.3 Proof of Proposition 24

#### Proof

Let  $\tau_{\text{tail}} = 2 \vee \sqrt{(D+3)/(2e)}$ . Given small enough  $\delta > 0$  as described below, we have

$$\begin{aligned}
 & \int_{\substack{\|\mathbf{x}-\mu_t\mathbf{y}\|_\infty \geq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} p_0(\mathbf{y})\phi_{\sigma_t}(\mathbf{x}-\mu_t\mathbf{y})d\mathbf{y} \\
 & \leq K \int_{\|\mathbf{x}-\mu_t\mathbf{y}\|_\infty \geq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)}} \phi_{\sigma_t}(\mathbf{x}-\mu_t\mathbf{y})d\mathbf{y} = K\mu_t^{-D} \int_{\|\mathbf{z}\|_\infty \geq \tau_{\text{tail}}\sqrt{\log(1/\delta)}} \phi_1(\mathbf{z})d\mathbf{z} \\
 & \leq K\mu_t^{-D} \sum_{i=1}^D \int_{|z_i| \geq \tau_{\text{tail}}\sqrt{\log(1/\delta)}} \phi(z_i)dz_i \leq 2KD\mu_t^{-D}\delta^{\tau_{\text{tail}}^2/2}
 \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t > 0$ , where the last inequality holds by the tail probability of the standard normal distribution. Also, for  $i \in [D]$ , we have

$$\begin{aligned}
 & \left| \int_{\substack{\|\mathbf{x}-\mu_t\mathbf{y}\|_\infty \geq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} \left( \frac{\mu_t y_i - x_i}{\sigma_t} \right) p_0(\mathbf{y})\phi_{\sigma_t}(\mathbf{x}-\mu_t\mathbf{y})d\mathbf{y} \right| \\
 & \leq K\mu_t^{-D} \int_{\|\mathbf{z}\|_\infty \geq \tau_{\text{tail}}\sqrt{\log(1/\delta)}} |z_i| \phi_1(\mathbf{z})d\mathbf{z} \leq K\mu_t^{-D} \sum_{j=1}^D \int_{|z_j| \geq \tau_{\text{tail}}\sqrt{\log(1/\delta)}} |z_j| \phi_1(\mathbf{z})d\mathbf{z} \\
 & = K\mu_t^{-D} \left\{ (D-1)\mathbb{E}[|Z|] \int_{|z| \geq \tau_{\text{tail}}\sqrt{\log(1/\delta)}} \phi(z)dz + \int_{|z| \geq \tau_{\text{tail}}\sqrt{\log(1/\delta)}} |z| \phi(z)dz \right\} \\
 & \leq K\mu_t^{-D} \left\{ 2(D-1)\sqrt{2/\pi}\delta^{\tau_{\text{tail}}^2/2} + \sqrt{\mathbb{E}[Z^2]}\sqrt{\mathbb{P}\left(|Z| \geq \tau_{\text{tail}}\sqrt{\log(1/\delta)}\right)} \right\} \\
 & \leq K\mu_t^{-D} \left\{ 2(D-1)\sqrt{2/\pi} + \sqrt{2} \right\} \delta^{\tau_{\text{tail}}^2/4},
 \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t > 0$ , where  $Z$  denotes the one-dimensional standard normal random variable and the second inequality holds by the Cauchy-Schwarz inequality. Since  $\mu_t^{-D} \leq 2^D$  for  $0 \leq t \leq (2\bar{\tau})^{-1}$ ,

$$\begin{aligned}
 & \left| p_t(\mathbf{x}) - \int_{\substack{\|\mathbf{x}-\mu_t\mathbf{y}\|_\infty \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} p_0(\mathbf{y})\phi_{\sigma_t}(\mathbf{x}-\mu_t\mathbf{y})d\mathbf{y} \right| \leq KD2^{D+1}\delta^{\tau_{\text{tail}}^2/2}, \\
 & \left\| \sigma_t \nabla p_t(\mathbf{x}) - \int_{\substack{\|\mathbf{x}-\mu_t\mathbf{y}\|_\infty \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} \left( \frac{\mu_t\mathbf{y}-\mathbf{x}}{\sigma_t} \right) p_0(\mathbf{y})\phi_{\sigma_t}(\mathbf{x}-\mu_t\mathbf{y})d\mathbf{y} \right\|_\infty \\
 & \leq K2^D \left\{ 2(D-1)\sqrt{2/\pi} + \sqrt{2} \right\} \delta^{\tau_{\text{tail}}^2/4}
 \end{aligned} \tag{63}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 < t \leq (2\bar{\tau})^{-1}$ . For  $0 < t \leq (2\bar{\tau})^{-1}$  and  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$  with  $\|\mathbf{x}\|_\infty \geq \mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}$ , we have

$$\begin{aligned} \|\mathbf{y}\|_\infty &\geq \frac{\|\mathbf{x}\|_\infty - \|\mathbf{x} - \mu_t \mathbf{y}\|_\infty}{\mu_t} \geq 1 - \left( \frac{\tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}} + \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}}{\mu_t} \right) \\ &\geq 1 - 2 \left[ \tau_x \left\{ \log(1/\sqrt{2\bar{\tau}t}) \right\}^{-\tau_{\text{bd}}} + \tau_{\text{tail}} \sqrt{2\bar{\tau}t \log(1/\delta)} \right], \end{aligned}$$

where the last inequality holds by (27). For  $0 < t \leq \delta^{\tau_t}$  and small enough  $\delta$  so that  $\delta^{\tau_t} \leq (2\bar{\tau})^{-1}$ , the last display is bounded by

$$1 - 2 \left[ \tau_x \left\{ \log(1/\sqrt{2\bar{\tau}\delta^{\tau_t}}) \right\}^{-\tau_{\text{bd}}} + \tau_{\text{tail}} \sqrt{2\bar{\tau}\delta^{\tau_t} \log(1/\delta)} \right].$$

Moreover, the last display is lower bounded by  $1 - 2D_1$  for small enough  $\delta$ , where

$$D_1 = \left( 2 \left[ 2 \{\log(1/\delta)\}^{\tilde{\tau}_{\text{bd}}} \vee 4 \right] + 2 \right)^{-1}.$$

Then,  $D_1 \leq (\{\log(1/\delta)\}^{-\tilde{\tau}_{\text{bd}}}/2) \wedge (1/4)$  and  $D_1^{-1} \in 2\mathbb{N}$ . Let  $\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(D_2)} \in \mathbb{R}^D$  be distinct vectors satisfying that

$$\left\{ \mathbf{y}^{(1)}, \dots, \mathbf{y}^{(D_2)} \right\} = \left\{ D_1(n_1, \dots, n_D)^\top : n_i \in \mathbb{Z}, i \in [D] \right\} \cap \left\{ \mathbf{y} \in \mathbb{R}^D : \|\mathbf{y}\|_\infty = 1 - D_1 \right\},$$

where  $D_2 = (2/D_1 - 1)^D - (2/D_1 - 3)^D$ . Let  $\mathcal{Y}_i = \{\mathbf{y} \in \mathbb{R}^D : \|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1\}$  for  $i \in [D_2]$ . For any  $i \in [D_2]$  and  $\mathbf{y} \in \mathcal{Y}_i$ , we have  $1 - 2D_1 \leq \|\mathbf{y}\|_\infty \leq 1$  and  $1 - 2D_1 \leq \|\mathbf{y}^{(i)}\|_\infty \leq 1$ . Assume that the density  $p_0$  satisfies

$$\sup_{\boldsymbol{\alpha} \in \mathbb{N}^D} \sup_{1 - \{\log(1/\delta)\}^{-\tilde{\tau}_{\text{bd}}} \leq \|\mathbf{x}\|_\infty \leq 1} |(\mathbf{D}^{\boldsymbol{\alpha}} p_0)(\mathbf{x})| \leq K.$$

With small enough  $\delta$  so that  $D_3 = \lceil \log_{4/e}(1/\delta) \rceil + 1 \geq 2$ , Taylor's theorem for multivariate function implies that

$$p_0(\mathbf{y}) = \sum_{0 \leq \mathbf{k} < D_3} \frac{(\mathbf{D}^{\mathbf{k}} p_0)(\mathbf{y}^{(i)})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} + \sum_{\mathbf{k} = D_3} \frac{(\mathbf{D}^{\mathbf{k}} p_0)(\xi \mathbf{y}^{(i)} + (1 - \xi) \mathbf{y})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}}$$

for a suitable  $\xi \in [0, 1]$  and  $i \in [D_2]$ ,  $\mathbf{y} \in \mathcal{Y}_i$ , where  $(\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} = \prod_{j=1}^D (y_j - y_j^{(i)})^{k_j}$ ,  $\mathbf{k}! = \prod_{j=1}^D k_j!$  and  $k. = \|\mathbf{k}\|_1$ . A simple calculation yields that

$$\begin{aligned} &\left| p_0(\mathbf{y}) - \sum_{0 \leq \mathbf{k} < D_3} \frac{(\mathbf{D}^{\mathbf{k}} p_0)(\mathbf{y}^{(i)})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \right| \cdot 1_{\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1\}} \\ &\leq \sum_{\mathbf{k} = D_3} K \prod_{j=1}^D \left( \frac{e D_1}{k_j} \right)^{k_j} \leq K (D_3 + 1)^D \left( \frac{e}{4} \right)^{D_3} \end{aligned}$$

for  $\mathbf{y} \in \mathbb{R}^D$  and  $i \in [D_2]$  because  $k! \geq k^k e^{-k}$  for any  $k \in \mathbb{Z}_{\geq 0}$  and  $0 < D_1 \leq 1/4$ . Since  $D_3 \geq \log \delta / \log(e/4)$ ,  $(e/4)^{D_3} \leq \delta$ . Then, the last display is further bounded by

$$K \left( \lfloor \log_{4/e}(1/\delta) \rfloor + 2 \right)^D \delta \leq K 3^D \delta \left\{ \frac{\log(1/\delta)}{\log(4/e)} \right\}^D.$$

Since  $\mathcal{Y}_1, \dots, \mathcal{Y}_{D_2}$  are mutually disjoint except on a set of Lebesgue measure zero and  $\bigcup_{i=1}^{D_2} \mathcal{Y}_i = \{\mathbf{y} \in \mathbb{R}^D : 1 - 2D_1 \leq \|\mathbf{y}\|_\infty \leq 1\}$ , we have

$$\begin{aligned} & \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} g(\mathbf{y}) d\mathbf{y} = \sum_{i=1}^{D_2} \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1}} g(\mathbf{y}) d\mathbf{y} \\ & = \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} g(\mathbf{y}) \cdot \mathbf{1}\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1\} d\mathbf{y} \end{aligned}$$

for any continuous function  $g : \mathbb{R}^D \rightarrow \mathbb{R}$ ,  $\|\mathbf{x}\|_\infty \geq \mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $0 < t \leq \delta^{\tau_t}$ . Combining (63) with the last two displays, we have

$$\begin{aligned} & \left| p_t(\mathbf{x}) - \sum_{i=1}^{D_2} \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1}} \left\{ \sum_{0 \leq k < D_3} \frac{(\mathbf{D}^k p_0)(\mathbf{y}^{(i)})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \right\} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| \\ & \leq K D 2^{D+1} \delta^{\tau_{\text{tail}}^2/2} + K 3^D \delta \left\{ \frac{\log(1/\delta)}{\log(e/4)} \right\}^D \\ & \quad \cdot \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) \cdot \mathbf{1}\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1\} d\mathbf{y} \\ & = K D 2^{D+1} \delta^{\tau_{\text{tail}}^2/2} + K 3^D \delta \left\{ \frac{\log(1/\delta)}{\log(4/e)} \right\}^D \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \geq \mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $0 < t \leq \delta^{\tau_t}$ . Moreover, the last display is bounded by

$$K D 2^{D+1} \delta^{\tau_{\text{tail}}^2/2} + K 6^D \delta \left\{ \frac{\log(1/\delta)}{\log(4/e)} \right\}^D \quad (64)$$

because  $\int_{\mathbb{R}^D} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} = \mu_t^{-D}$  and  $\mu_t^{-D} \leq 2^D$  by (27). Also, we have

$$\begin{aligned} & \left\| \sigma_t \nabla p_t(\mathbf{x}) - \sum_{i=1}^{D_2} \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1}} \left\{ \sum_{0 \leq k < D_3} \frac{(\mathbf{D}^k p_0)(\mathbf{y}^{(i)})}{\mathbf{k}!} \left( \frac{\mu_t \mathbf{y} - \mathbf{x}}{\sigma_t} \right) (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \right\} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right\|_\infty \\ & \leq K 2^D \left\{ 2(D-1)\sqrt{2/\pi} + \sqrt{2} \right\} \delta^{\tau_{\text{tail}}^2/4} + K 3^D \delta \left\{ \frac{\log(1/\delta)}{\log(4/e)} \right\}^D \\ & \quad \cdot \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq 1}} \sum_{i=1}^{D_2} \left\| \frac{\mu_t \mathbf{y} - \mathbf{x}}{\sigma_t} \right\|_\infty \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) \cdot \mathbf{1}\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1\} d\mathbf{y} \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \geq \mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $0 < t \leq \delta^{\tau_x}$ . Moreover, the last display is bounded by

$$K2^D \left\{ 2(D-1)\sqrt{2/\pi} + \sqrt{2} \right\} \delta^{\tau_{\text{tail}}^2/4} + 2K\tau_{\text{tail}}6^D \{\log(4/e)\}^{-D} \delta \{\log(1/\delta)\}^{D+1/2} \quad (65)$$

because  $\int_{\mathbb{R}^D} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} = \mu_t^{-D}$  and  $\mu_t^{-D} \leq 2^D$  by (27).

For  $x, y \in \mathbb{R}$  and  $t > 0$ , Taylor's theorem yields that

$$\left| \exp\left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right) - \sum_{l=0}^{D_4-1} \frac{1}{l!} \left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right)^l \right| \leq \frac{1}{D_4!} \left(\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right)^{D_4},$$

where  $D_4 = \lfloor 2e\tau_{\text{tail}}^2 \log(1/\delta) \rfloor + 1$  with small enough  $\delta$  so that  $D_4 \geq 1$ . For  $|x - \mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)}$  and  $t \geq 0$ , the last display is further bounded by

$$\left(\frac{e\tau_{\text{tail}}^2 \log(1/\delta)}{D_4}\right)^{D_4} \leq 2^{-D_4} \leq \delta^{2e\tau_{\text{tail}}^2 \log 2} \leq \delta^{e\tau_{\text{tail}}^2},$$

where the last inequality holds because  $1/2 \leq \log 2$  and  $0 < \delta < 1$ . Then,

$$\begin{aligned} & \left| \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq \tilde{\tau}}} \left(\frac{\mu_t y - x}{\sigma_t}\right)^m (y - \tilde{y})^k \exp\left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right) dy \right. \\ & \quad \left. - \sum_{l=0}^{D_4-1} \frac{1}{l!} \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq D_1}} \left(\frac{\mu_t y - x}{\sigma_t}\right)^m (y - \tilde{y})^k \left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right)^l dy \right| \\ & \leq \delta^{e\tau_{\text{tail}}^2} \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq D_1}} \left|\frac{\mu_t y - x}{\sigma_t}\right|^m |y - \tilde{y}|^k dy \\ & \leq \delta^{e\tau_{\text{tail}}^2} \int_{|y| \leq 1} D_1^k \left\{ \tau_{\text{tail}}\sqrt{\log(1/\delta)} \right\}^m dy \leq \delta^{e\tau_{\text{tail}}^2} \left\{ \tau_{\text{tail}}\sqrt{\log(1/\delta)} \right\}^m \end{aligned}$$

for any  $x, \tilde{y} \in \mathbb{R}$  with  $|\tilde{y}| = 1 - D_1, t \geq 0, k \in \mathbb{Z}_{\geq 0}$  and  $m \in \{0, 1\}$ , where the last inequality holds because  $D_1 < 1$ . Moreover,

$$\begin{aligned} & \left| \sum_{l=0}^{D_4-1} \frac{1}{l!} \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq D_1}} \left(\frac{\mu_t y - x}{\sigma_t}\right)^m (y - \tilde{y})^k \left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right)^l dy \right| \\ & \leq \left(1 + \delta^{e\tau_{\text{tail}}^2}\right) \left\{ \tau_{\text{tail}}\sqrt{\log(1/\delta)} \right\}^m \end{aligned}$$

for any  $x, \tilde{y} \in \mathbb{R}$  with  $|\tilde{y}| = 1 - D_1, t \geq 0, k \in \mathbb{Z}_{\geq 0}$  and  $m \in \{0, 1\}$  because

$$\begin{aligned} & \left| \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq D_1}} \left(\frac{\mu_t y - x}{\sigma_t}\right)^m (y - \tilde{y})^k \exp\left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right) dy \right| \\ & \leq D_1^k \left\{ \tau_{\text{tail}}\sqrt{\log(1/\delta)} \right\}^m \int_{|y| \leq 1} 1 dy \leq \left\{ \tau_{\text{tail}}\sqrt{\log(1/\delta)} \right\}^m. \end{aligned}$$

Note that  $|\prod_{j=1}^D x_j - \prod_{j=1}^D \tilde{x}_j| \leq DC^{D-1} \|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty$  for any  $\mathbf{x}, \tilde{\mathbf{x}} \in [-C, C]^D$ . Since the last two displays are bounded by  $2\{\tau_{\text{tail}}\sqrt{\log(1/\delta)}\}^m$ , we have

$$\begin{aligned} & \left| \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq D_1}} \left( \frac{\mu_t y_h - x_h}{\sigma_t} \right)^m (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} - \right. \\ & \left. \prod_{j=1}^D \sum_{l=0}^{D_4-1} \frac{1}{l! \sqrt{2\pi} \sigma_t} \int_{\substack{|x_j - \mu_t y_j| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y_j - y_j^{(i)}| \leq D_1}} \left( \frac{\mu_t y_h - x_h}{\sigma_t} \right)^{m \cdot 1\{h=j\}} (y_j - y_j^{(i)})^{k_j} \left( -\frac{(x_j - \mu_t y_j)^2}{2\sigma_t^2} \right)^l dy_j \right| \\ & \leq (2\pi\sigma_t^2)^{-\frac{D}{2}} D 2^{D-1} \delta e^{\tau_{\text{tail}}^2} \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^{mD} \end{aligned} \quad (66)$$

for  $\mathbf{x} \in \mathbb{R}^D$ ,  $t \geq 0$ ,  $h \in [D]$ ,  $i \in [D_2]$ ,  $j \in [D]$ ,  $\mathbf{k} \in \mathbb{Z}_{\geq 0}^D$  and  $m \in \{0, 1\}$  with small enough  $\delta$  so that  $\tau_{\text{tail}}\sqrt{\log(1/\delta)} > 1$ . With  $m = 0$  in the last display, the last integral satisfies that

$$\begin{aligned} & \frac{1}{l! \sqrt{2\pi} \sigma_t} \int_{\substack{|x_j - \mu_t y_j| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y_j - y_j^{(i)}| \leq D_1}} (y_j - y_j^{(i)})^{k_j} \left( -\frac{(x_j - \mu_t y_j)^2}{2\sigma_t^2} \right)^l dy_j \\ & = \frac{\mu_t^{-1}}{l! \sqrt{2\pi}} \int_{\substack{|z_j| \leq \tau_{\text{tail}} \sqrt{\log(1/\delta)} \\ |\mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)}| \leq D_1}} \left( \mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)} \right)^{k_j} z_j^{2l} (-2)^{-l} dz_j \\ & = \frac{(-2)^{-l} \mu_t^{-1}}{l! \sqrt{2\pi}} \int_{\substack{|z_j| \leq \tau_{\text{tail}} \sqrt{\log(1/\delta)} \\ |\mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)}| \leq D_1}} \sum_{r_j=0}^{k_j} \binom{k_j}{r_j} (\mu_t^{-1} \sigma_t)^{r_j} (\mu_t^{-1} x_j - y_j^{(i)})^{k_j - r_j} z_j^{r_j + 2l} dz_j \\ & = \frac{(-2)^{-l} \mu_t^{-k_j - 1}}{l! \sqrt{2\pi}} \sum_{r_j=0}^{k_j} \binom{k_j}{r_j} \sigma_t^{r_j} (x_j - \mu_t y_j^{(i)})^{k_j - r_j} \left( \frac{\bar{z}_{i,j}^{r_j + 2l + 1} - \underline{z}_{i,j}^{r_j + 2l + 1}}{r_j + 2l + 1} \right) \stackrel{\text{def}}{=} P_{i,j,k_j,l}(x_j, t), \end{aligned}$$

where

$$\begin{aligned} \bar{z}_{i,j} &= \min \left( \max \left( \frac{\mu_t (y_j^{(i)} + D_1) - x_j}{\sigma_t}, -\tau_{\text{tail}} \sqrt{\log(1/\delta)} \right), \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right), \\ \underline{z}_{i,j} &= \min \left( \max \left( \frac{\mu_t (y_j^{(i)} - D_1) - x_j}{\sigma_t}, -\tau_{\text{tail}} \sqrt{\log(1/\delta)} \right), \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right). \end{aligned}$$

Combining (27), (64) and (66) with the last two displays, we have

$$\begin{aligned} & |p_t(\mathbf{x}) - g_t(\mathbf{x})| \\ & \leq K D 2^{D+1} \delta \tau_{\text{tail}}^{2/2} + K 6^D \delta \left\{ \frac{\log(1/\delta)}{\log(4/e)} \right\}^D \\ & \quad + \sum_{i=1}^{D_2} \sum_{0 \leq k < D_3} \left| \frac{(D^{\mathbf{k}} p_0)(\mathbf{y}^{(i)})}{\mathbf{k}!} \right| (2\pi\sigma_t^2)^{-\frac{D}{2}} D 2^{D-1} \delta e^{\tau_{\text{tail}}^2} \\ & \leq D_5 \left[ \delta \tau_{\text{tail}}^{2/2} + \delta \{\log(1/\delta)\}^D + \delta e^{\tau_{\text{tail}}^2} \delta^{-D/2} \{\log(1/\delta)\}^{D\tilde{\tau}_{\text{bd}} + D} \right] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \geq \mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $\delta \leq t \leq \delta^{\tau_t}$ , where  $D_5 = D_5(D, K, \underline{\tau}, \tau_{\text{tail}})$  and  $g_t : \mathbb{R}^D \rightarrow \mathbb{R}$  is a function such that

$$g_t(\mathbf{x}) = \sum_{i=1}^{D_2} \sum_{0 \leq k < D_3} \left\{ (D^{\mathbf{k}} p_0)(\mathbf{y}^{(i)}) \right\} \prod_{j=1}^D \sum_{l=0}^{D_4-1} \frac{P_{i,j,k_j,l}(x_j, t)}{k_j!}, \quad \mathbf{x} \in \mathbb{R}^D.$$

Since  $\tau_{\text{tail}} \geq 2 \vee \sqrt{(D+3)/(2e)}$ , we have

$$|p_t(\mathbf{x}) - g_t(\mathbf{x})| \leq 3D_5 \delta \{\log(1/\delta)\}^D \quad (67)$$

for small enough  $\delta$ . Similarly, with  $m = 1$  and  $h = j$  in (66), the last integral in (66) satisfies that

$$\begin{aligned} & \frac{1}{l! \sqrt{2\pi} \sigma_t} \int_{\substack{|x_j - \mu_t y_j| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y_j - y_j^{(i)}| \leq D_1}} \left( \frac{\mu_t y_j - x_j}{\sigma_t} \right) (y_j - y_j^{(i)})^{k_j} \left( -\frac{(x_j - \mu_t y_j)^2}{2\sigma_t^2} \right)^l dy_j \\ &= \frac{\mu_t^{-1}}{l! \sqrt{2\pi}} \int_{\substack{|z_j| \leq \tau_{\text{tail}} \sqrt{\log(1/\delta)} \\ |\mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)}| \leq D_1}} \left( \mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)} \right)^{k_j} z_j^{2l+1} (-2)^{-l} dz_j \\ &= \frac{(-2)^{-l} \mu_t^{-k_j-1}}{l! \sqrt{2\pi}} \sum_{r_j=0}^{k_j} \binom{k_j}{r_j} \sigma_t^{r_j} \left( x_j - \mu_t y_j^{(i)} \right)^{k_j-r_j} \left( \frac{\bar{z}_{i,j}^{r_j+2l+2} - \underline{z}_{i,j}^{r_j+2l+2}}{r_j+2l+2} \right) \stackrel{\text{def}}{=} \tilde{P}_{i,j,k_j,l}(x_j, t). \end{aligned}$$

Combining (27), (65) and (66) with the last display, we have

$$\begin{aligned} & \left| \sigma_t (\nabla p_t(\mathbf{x}))_h - \tilde{g}_t^{(h)}(\mathbf{x}) \right| \\ & \leq K 2^D \left\{ 2(D-1) \sqrt{2/\pi} + \sqrt{2} \right\} \delta^{\tau_{\text{tail}}^2/4} + 2K \tau_{\text{tail}} 6^D \{\log(4/e)\}^{-D} \delta \{\log(1/\delta)\}^{D+1/2} \\ & \quad + \sum_{i=1}^{D_2} \sum_{0 \leq k < D_3} \left| \frac{(D^{\mathbf{k}} p_0)(\mathbf{y}^{(i)})}{\mathbf{k}!} \right| (2\pi \sigma_t^2)^{-\frac{D}{2}} D 2^{D-1} \delta^{e\tau_{\text{tail}}^2} \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^D \\ & \leq D_6 \left[ \delta^{\tau_{\text{tail}}^2/4} + \delta \{\log(1/\delta)\}^{D+1/2} + \delta^{e\tau_{\text{tail}}^2-D/2} \{\log(1/\delta)\}^{D(\tilde{\tau}_{\text{bd}}+3/2)} \right], \quad h \in [D] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \geq \mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tau_{\text{bd}}}$  and  $\delta \leq t \leq \delta^{\tau_t}$ , where  $D_6 = D_6(D, K, \tau_{\text{tail}}, \underline{\tau})$  and  $\tilde{g}_t^{(h)} : \mathbb{R}^D \rightarrow \mathbb{R}$ ,  $h \in [D]$  is a function such that

$$\tilde{g}_t^{(h)}(\mathbf{x}) = \sum_{i=1}^{D_2} \sum_{0 \leq k < D_3} \left\{ (D^{\mathbf{k}} p_0)(\mathbf{y}^{(i)}) \right\} \left\{ \prod_{\substack{j=1 \\ j \neq h}}^D \sum_{l=0}^{D_4-1} \frac{P_{i,j,k_j,l}(x_j, t)}{k_j!} \right\} \left\{ \sum_{l=0}^{D_4-1} \frac{\tilde{P}_{i,h,k_h,l}(x_h, t)}{k_h!} \right\}.$$

Since  $\tau_{\text{tail}} \geq 2 \vee \sqrt{(D+3)/(2e)}$ , we have

$$\left| \sigma_t (\nabla p_t(\mathbf{x}))_h - \tilde{g}_t^{(h)}(\mathbf{x}) \right| \leq 3D_6 \delta \{\log(1/\delta)\}^D, \quad h \in [D] \quad (68)$$

for small enough  $\delta$ .

Let  $0 < \tilde{\delta} < \delta$  be a small enough value as described below. With  $\tilde{\delta}^2 < 1/2$ , Lemma 18 implies that there exist neural networks  $f_\mu \in \mathcal{F}_{\text{NN}}(L_\mu, \mathbf{d}_\mu, s_\mu, M_\mu)$ ,  $f_\sigma \in \mathcal{F}_{\text{NN}}(L_\sigma, \mathbf{d}_\sigma, s_\sigma, M_\sigma)$  with

$$\begin{aligned} L_\mu, L_\sigma &\leq C_{N,4} \{\log(1/\tilde{\delta})\}^2, & \|\mathbf{d}_\mu\|_\infty, \|\mathbf{d}_\sigma\|_\infty &\leq C_{N,4} \{\log(1/\tilde{\delta})\}^2 \\ s_\mu, s_\sigma &\leq C_{N,4} \{\log(1/\tilde{\delta})\}^3, & M_\mu, M_\sigma &\leq C_{N,4} \log(1/\tilde{\delta}) \end{aligned}$$

such that  $|\mu_t - f_\mu(t)| \leq \tilde{\delta}$  and  $|\sigma_t - f_\sigma(t)| \leq \tilde{\delta}$  for  $t \geq \tilde{\delta}$ , where  $C_{N,4}$  is the constant in Lemma 18. Also, Lemma 19 implies that there exist a neural network  $f_{\text{rec}} \in \mathcal{F}_{\text{NN}}(L_{\text{rec}}, \mathbf{d}_{\text{rec}}, s_{\text{rec}}, M_{\text{rec}})$  with

$$\begin{aligned} L_{\text{rec}} &\leq C_{N,5} \{\log(1/\tilde{\delta})\}^2, & \|\mathbf{d}_{\text{rec}}\|_\infty &\leq C_{N,5} \{\log(1/\tilde{\delta})\}^3 \\ s_{\text{rec}} &\leq C_{N,5} \{\log(1/\tilde{\delta})\}^4, & M_{\text{rec}} &\leq C_{N,5} \tilde{\delta}^{-2} \end{aligned}$$

such that  $|1/x - f_{\text{rec}}(x)| \leq \tilde{\delta}$  for any  $x \in [\tilde{\delta}, 1/\tilde{\delta}]$ , where  $C_{N,5}$  is the constant in Lemma 19. Since  $\sigma_t - \tilde{\delta} \leq f_\sigma(t) \leq \sigma_t + \tilde{\delta}$  for  $t \geq \tilde{\delta}$  and  $\sqrt{\tau t} \leq \sigma_t \leq 1$  for  $t \geq \delta$ , we have  $\delta \leq f_\sigma(t) \leq 2$  for  $t \geq \delta$  with small enough  $\tilde{\delta}$  so that  $\tilde{\delta} \leq \sqrt{\tau \tilde{\delta}} - \delta$  and  $\tilde{\delta} \leq 1$ . A simple calculation yields that

$$\begin{aligned} |1/\sigma_t - f_{\text{rec}}(f_\sigma(t))| &\leq |1/\sigma_t - 1/f_\sigma(t)| + |1/f_\sigma(t) - f_{\text{rec}}(f_\sigma(t))| \\ &\leq \{\sigma_t \wedge f_\sigma(t)\}^{-2} |\sigma_t - f_\sigma(t)| + \tilde{\delta} \leq (1 + \delta^{-2}) \tilde{\delta} \end{aligned} \tag{69}$$

for  $t \geq \delta$ . Lemma 14 implies that there exists a neural network

$$\tilde{f}_{\text{mult}}^{(k)} \in \mathcal{F}_{\text{NN}}(\tilde{L}_{\text{mult}}^{(k)}, \tilde{\mathbf{d}}_{\text{mult}}^{(k)}, \tilde{s}_{\text{mult}}^{(k)}, \tilde{M}_{\text{mult}}^{(k)}), \quad k \geq 2$$

with

$$\begin{aligned} \tilde{L}_{\text{mult}}^{(k)} &\leq C_{N,1} \log k \{\log(1/\tilde{\delta}) + \log(1/\delta)\}, & \tilde{\mathbf{d}}_{\text{mult}}^{(k)} &= (k, 48k, \dots, 48k, 1)^\top, \\ \tilde{s}_{\text{mult}}^{(2)} &\leq C_{N,1} k \{\log(1/\tilde{\delta}) + \log(1/\delta)\}, & \tilde{M}_{\text{mult}}^{(k)} &= \delta^{-k} \end{aligned}$$

such that

$$\left| \tilde{f}_{\text{mult}}^{(k)}(\tilde{x}_1, \dots, \tilde{x}_k) - \prod_{i=1}^k x_i \right| \leq \tilde{\delta} + k\delta^{-(k-1)}\tilde{\epsilon} \tag{70}$$

for any  $\mathbf{x} = (x_1, \dots, x_k) \in \mathbb{R}^k$  with  $\|\mathbf{x}\|_\infty \leq \delta^{-1}$  and  $\tilde{\mathbf{x}} = (\tilde{x}_1, \dots, \tilde{x}_k) \in \mathbb{R}^k$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ , where  $0 < \tilde{\epsilon} \leq 1$  and  $C_{N,1}$  is the constant in Lemma 14. Let

$$f_{\text{clip}} \in \mathcal{F}_{\text{NN}}(2, (1, 2, 1)^\top, 7, \tau_{\text{tail}} \sqrt{\log(1/\delta)})$$

be the neural network in Lemma 15 such that  $f_{\text{clip}}(x) = (x \vee -\tau_{\text{tail}} \sqrt{\log(1/\delta)}) \wedge \tau_{\text{tail}} \sqrt{\log(1/\delta)}$  for  $x \in \mathbb{R}$ . For  $i \in [D_2]$  and  $j \in [D]$ , consider functions  $\bar{f}_{i,j}, \underline{f}_{i,j} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} \bar{f}_{i,j}(x, t) &= f_{\text{clip}} \left( \tilde{f}_{\text{mult}}^{(2)} \left( f_{\text{rec}}(f_\sigma(t)), \{y_j^{(i)} + D_1\} f_\mu(t) - x \right) \right), \\ \underline{f}_{i,j}(x, t) &= f_{\text{clip}} \left( \tilde{f}_{\text{mult}}^{(2)} \left( f_{\text{rec}}(f_\sigma(t)), \{y_j^{(i)} - D_1\} f_\mu(t) - x \right) \right), \end{aligned}$$

for  $x, t \in \mathbb{R}$ . Note that  $|y_j^{(i)} + D_1| \leq 1$  and  $|y_j^{(i)} - D_1| \leq 1$  for  $i \in [D_2]$ . Combining (69) and (70) with the last display, both  $|\bar{z}_{i,j} - \bar{f}_{i,j}(x, t)|$  and  $|\underline{z}_{i,j} - \underline{f}_{i,j}(x, t)|$  are bounded by

$$\tilde{\delta} + 2\delta^{-1}(1 + \delta^{-2})\tilde{\delta} \leq 5\delta^{-3}\tilde{\delta} \quad (71)$$

for  $|x| \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \delta^{\tau_x}$  with small enough  $\delta$  so that  $|(y_j^{(i)} + D_1)\mu_t - x|$ ,  $|(y_j^{(i)} - D_1)\mu_t - x|$  and  $1/\sigma_t$  are upper bounded by  $\delta^{-1}$ . Since  $\mu_t - \tilde{\delta} \leq f_\mu(t) \leq \mu_t + \tilde{\delta}$  for  $t \geq \tilde{\delta}$ , we have  $1/4 \leq 1/2 - \tilde{\delta} \leq f_\mu(t) \leq 1 + \tilde{\delta} \leq 2$  and  $1/4 \leq \mu_t \leq 2$  for  $\delta \leq t \leq D_1$  with small enough  $\tilde{\delta}$  by (27). A simple calculation yields that

$$\begin{aligned} |1/\mu_t - f_{\text{rec}}(f_\mu(t))| &\leq |1/\mu_t - 1/f_\mu(t)| + |1/f_\mu(t) - f_{\text{rec}}(f_\mu(t))| \\ &\leq \{\mu_t \wedge f_\mu(t)\}^{-2} |\mu_t - f_\mu(t)| + \tilde{\delta} \leq 17\tilde{\delta} \end{aligned} \quad (72)$$

for  $\delta \leq t \leq \delta^{\tau_x}$ . For any  $i \in [D_2], j \in [D], k \in \{0, \dots, D_3 - 1\}$ , consider functions  $f_{i,j,k}, \tilde{f}_{i,j,k} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} f_{i,j,k}(x, t) &= \sum_{l=0}^{D_4-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{(-2)^{-l}}{k!l!\sqrt{2\pi}(r+2l+1)} \right\} \left\{ \bar{f}_{i,j,k,l,r,r+2l+1} - \underline{f}_{i,j,k,l,r,r+2l+1} \right\}, \\ \tilde{f}_{i,j,k}(x, t) &= \sum_{l=0}^{D_4-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{(-2)^{-l}}{k!l!\sqrt{2\pi}(r+2l+2)} \right\} \left\{ \bar{f}_{i,j,k,l,r,r+2l+2} - \underline{f}_{i,j,k,l,r,r+2l+2} \right\}, \end{aligned}$$

for  $x, t \in \mathbb{R}$ , where

$$\begin{aligned} \bar{f}_{i,j,k,l,r,s} &= \tilde{f}_{\text{mult}}^{(2k+s+1)} \left( f_{\text{rec}}(f_\mu(t)) \cdot \mathbf{1}_{k+1}, f_\sigma(t) \cdot \mathbf{1}_r, \left\{ x - f_\mu(t)y_j^{(i)} \right\} \cdot \mathbf{1}_{k-r}, \bar{f}_{i,j}(x, t) \cdot \mathbf{1}_s \right), \\ \underline{f}_{i,j,k,l,r,s} &= \tilde{f}_{\text{mult}}^{(2k+s+1)} \left( f_{\text{rec}}(f_\mu(t)) \cdot \mathbf{1}_{k+1}, f_\sigma(t) \cdot \mathbf{1}_r, \left\{ x - f_\mu(t)y_j^{(i)} \right\} \cdot \mathbf{1}_{k-r}, \underline{f}_{i,j}(x, t) \cdot \mathbf{1}_s \right), \end{aligned}$$

for  $s \in \{r+2l+1, r+2l+2\}$ . Combining (72), (69), (71) and (70) with the last two displays, the definition of  $P_{i,j,k,l}(x, t)$  and  $\tilde{P}_{i,j,k,l}(x, t)$  implies that

$$\begin{aligned} &\left| \sum_{l=0}^{D_4-1} \frac{P_{i,j,k,l}(x, t)}{k!} - f_{i,j,k}(x, t) \right| \\ &\leq \sum_{l=0}^{D_4-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{2^{-l+1}}{k!l!\sqrt{2\pi}(r+2l+2)} \right\} \left\{ \tilde{\delta} + 5(2k+r+2l+1)\delta^{-2k-r-2l-4}\tilde{\delta} \right\} \end{aligned}$$

and

$$\begin{aligned} &\left| \sum_{l=0}^{D_4-1} \frac{\tilde{P}_{i,j,k,l}(x, t)}{k!} - \tilde{f}_{i,j,k}(x, t) \right| \\ &\leq \sum_{l=0}^{D_4-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{2^{-l+1}}{k!l!\sqrt{2\pi}(r+2l+3)} \right\} \left\{ \tilde{\delta} + 5(2k+r+2l+2)\delta^{-2k-r-2l-5}\tilde{\delta} \right\} \end{aligned}$$

for  $i \in [D_2], j \in [D], k \in \{0, \dots, D_3 - 1\}, |x| \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \delta^{\tau_t}$  with small enough  $\delta$  so that  $\sigma_t, \mu_t^{-1}, |x - y_j^{(i)}|, \tau_{\text{tail}} \sqrt{\log(1/\delta)}$  are all upper bounded by  $\delta^{-1}$ . Since  $\sum_{r=0}^k \binom{k}{r} = 2^k$  and  $2^k/k! \leq 2$  for all  $k \in \mathbb{N}$ , the last two displays are bounded by

$$\sum_{l=0}^{D_4-1} \left( \frac{2^{-l+2}}{l! \sqrt{2\pi}(2l+1)} \right) \left\{ 1 + 5(3D_4 + 2l) \delta^{-3D_3-2l} \right\} \tilde{\delta} \leq \delta^{-D_7 \log(1/\delta)} \tilde{\delta}, \quad (73)$$

where  $D_7 = D_7(\tau_{\text{tail}})$ . For any  $i \in [D_2], j \in [D], k \in \{0, \dots, D_3 - 1\}, l \in \{0, \dots, D_4 - 1\}, |x| \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \delta^{\tau_t}$ , we have

$$\left| \frac{P_{i,j,k,l}(x,t)}{k!} \right| \leq \left\{ \frac{2^{-l-k}}{k! l! \sqrt{2\pi}(r+2l+1)} \sum_{r=0}^k \binom{k}{r} \right\} \left\{ 2\mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)} \right\}^k \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^{k+2l+1}$$

and

$$\left| \frac{\tilde{P}_{i,j,k,l}(x,t)}{k!} \right| \leq \left\{ \frac{2^{-l-k}}{k! l! \sqrt{2\pi}(r+2l+1)} \sum_{r=0}^k \binom{k}{r} \right\} \left\{ 2\mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)} \right\}^k \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^{k+2l+2}$$

by the definition of  $P_{i,j,k,l}(x)$  and  $\tilde{P}_{i,j,k,l}(x)$ . Since  $\sum_{r=0}^k \binom{k}{r} = 2^k$  and  $2^k/k! \leq 2$  for all  $k \in \mathbb{N}$ , the last two displays are bounded by  $\{D_8 \log(1/\delta)\}^{k+l+1}$ , where  $D_8 = D_8(\tau_{\text{tail}}, \tau_x)$ . Then,

$$\begin{aligned} \left| \sum_{l=0}^{D_4-1} \frac{P_{i,j,k,l}(x)}{k!} \right| &\leq D_4 \{D_8 \log(1/\delta)\}^{D_3+D_4-1} \leq \{\log(1/\delta)\}^{D_9 \log(1/\delta)} \quad \text{and} \\ \left| \sum_{l=0}^{D_4-1} \frac{\tilde{P}_{i,j,k,l}(x)}{k!} \right| &\leq D_4 \{D_8 \log(1/\delta)\}^{D_3+D_4-1} \leq \{\log(1/\delta)\}^{D_9 \log(1/\delta)} \end{aligned}$$

for  $i \in [D_2], j \in [D], k \in \{0, \dots, D_3 - 1\}, |x| \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \delta^{\tau_t}$ , where  $D_9 = D_9(\tau_{\text{tail}}, D_8)$ . Consider functions  $f, \tilde{f}^{(1)}, \dots, \tilde{f}^{(D)} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} f(\mathbf{x}, t) &= \sum_{i=1}^{D_2} \sum_{0 \leq k < D_3} \left\{ (D^{\mathbf{k}} p_0)(\mathbf{y}^{(i)}) \right\} f_{\text{mult}}^{(D)}(f_{i,1,k_1}(x_1, t), \dots, f_{i,D,k_D}(x_D, t)) \quad \text{and} \\ \tilde{f}^{(h)}(\mathbf{x}, t) &= \sum_{i=1}^{D_2} \sum_{0 \leq k < D_3} \left\{ (D^{\mathbf{k}} p_0)(\mathbf{y}^{(i)}) \right\} f_{\text{mult}}^{(D)} \left( \underbrace{\tilde{f}_{i,h,k_h}(x_h, t), f_{i,1,k_1}(x_1, t), \dots, f_{i,D,k_D}(x_D, t)}_{\text{without } f_{i,h,k_h}(x_h, t)} \right), \end{aligned}$$

where  $f_{\text{mult}}^{(D)} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}^{(D)}, \mathbf{d}_{\text{mult}}^{(D)}, s_{\text{mult}}^{(D)}, M_{\text{mult}}^{(D)})$  is the neural network in Lemma 14 with

$$\begin{aligned} L_{\text{mult}}^{(D)} &\leq C_{N,1} \log D [\log(1/\tilde{\delta}) + DD_9 \log(1/\delta) \log \log(1/\delta)], \quad \mathbf{d}_{\text{mult}}^{(D)} = (D, 48D, \dots, 48D, 1)^\top, \\ s_{\text{mult}}^{(D)} &\leq C_{N,1} D [\log(1/\tilde{\delta}) + D_9 \log(1/\delta) \log \log(1/\delta)], \quad M_{\text{mult}}^{(D)} = \{\log(1/\delta)\}^{DD_9 \log(1/\delta)} \end{aligned}$$

such that

$$\left| f_{\text{mult}}^{(D)}(\tilde{x}_1, \dots, \tilde{x}_D) - \prod_{i=1}^D x_i \right| \leq \tilde{\delta} + D \{\log(1/\delta)\}^{(D-1)D_9 \log(1/\delta)} \tilde{\epsilon}$$

for any  $\mathbf{x} = (x_1, \dots, x_D) \in \mathbb{R}^D$  with  $\|\mathbf{x}\|_\infty \leq \{\log(1/\delta)\}^{D_9 \log(1/\delta)}$  and  $\tilde{\mathbf{x}} = (\tilde{x}_1, \dots, \tilde{x}_D) \in \mathbb{R}^D$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ . Combining (73) with the last display, we have

$$\begin{aligned} & |f(\mathbf{x}, t) - g_t(\mathbf{x})| \\ & \leq \sum_{i=1}^{D_2} \sum_{0 \leq k < D_3} \left| (\mathbf{D}^{\mathbf{k}} p_0)(\mathbf{y}^{(i)}) \right| \left\{ 1 + D\delta^{-D_7 \log(1/\delta)} \{\log(1/\delta)\}^{(D-1)D_9 \log(1/\delta)} \right\} \tilde{\delta} \\ & \leq K D_2 D_3^D \left\{ 1 + D\delta^{-D_7 \log(1/\delta)} \{\log(1/\delta)\}^{(D-1)D_9 \log(1/\delta)} \right\} \tilde{\delta} \leq \delta^{-D_{10} \log(1/\delta)} \tilde{\delta} \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq D_1$ , where  $D_{10} = D_{10}(D, K, \tilde{\tau}_{\text{bd}}, D_7, D_9)$  is a large enough constant. Similarly, we have

$$\left| \tilde{f}^{(h)}(\mathbf{x}, t) - \tilde{g}_t^{(h)}(\mathbf{x}) \right| \leq \delta^{-D_{10} \log(1/\delta)} \tilde{\delta}, \quad h \in [D]$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \delta^{\tau_t}$ . Let  $\tilde{\delta} = \delta^{D_{10} \log(1/\delta) + 1}$ . Combining (67) and (68) with the last two displays, we have

$$\begin{aligned} |p_t(\mathbf{x}) - f(\mathbf{x}, t)| & \leq \delta + 3D_5 \delta \{\log(1/\delta)\}^D \leq (1 + 3D_5) \delta \{\log(1/\delta)\}^D \quad \text{and} \\ \left| \sigma_t (\nabla p_t(\mathbf{x}))_h - \tilde{f}^{(h)}(\mathbf{x}, t) \right| & \leq \delta + 3D_6 \delta \{\log(1/\delta)\}^D \leq (1 + 3D_6) \delta \{\log(1/\delta)\}^D, \quad h \in [D] \end{aligned}$$

for  $\mu_t - \tau_x \{\log(1/\sigma_t)\}^{-\tilde{\tau}_{\text{bd}}} \leq \|\mathbf{x}\|_\infty \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \delta^{\tau_t}$ . Note that

$$D_2 \leq D_{13} \{\log(1/\delta)\}^{D \tilde{\tau}_{\text{bd}}}, \quad D_3 \leq D_{13} \log(1/\delta), \quad D_4 \leq D_{13} \log(1/\delta),$$

where  $D_{13} = D_{13}(D, \tau_{\text{tail}})$ . Consider a function  $\mathbf{f} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{D+1}$  such that

$$\mathbf{f}(\mathbf{x}, t) = (\tilde{f}^{(1)}(\mathbf{x}, t), \dots, \tilde{f}^{(D)}(\mathbf{x}, t), f(\mathbf{x}, t))^\top$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . Lemma 9, Lemma 10, Lemma 11 and Lemma 12 implies that  $\mathbf{f} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, M)$  with

$$\begin{aligned} L & \leq D_{11} \{\log(1/\delta)\}^4, \quad \|\mathbf{d}\|_\infty \leq D_{11} \{\log(1/\delta)\}^{7+D \tilde{\tau}_{\text{bd}}+D}, \\ s & \leq D_{11} \{\log(1/\delta)\}^{11+D \tilde{\tau}_{\text{bd}}+D}, \quad M \leq \exp(D_{11} \{\log(1/\delta)\}^2), \end{aligned}$$

where  $D_{11} = D_{11}(D, K, \tau_{\text{tail}}, C_{N,1}, C_{N,4}, C_{N,5}, D_9, D_{13})$ . The assertion follows by re-defining the constants. ■

## B.4 Proof of Proposition 25

**Proof** Let

$$\tau_t = \bar{\tau}^{-1} \quad \text{and} \quad \tau_{\text{tail}} = \left\{ 4(D\bar{\tau}\tau_t + 1) \vee \left( \frac{D+1}{e} \right) \right\}^{\frac{1}{2}}.$$

Let  $t_* > 0$  and  $0 < \delta < 1$  be small enough values as described below. By the Markov property of  $(\mathbf{X}_t)_{t \geq 0}$ , we have

$$p_{t_*+t}(\mathbf{x}) = \int_{\mathbb{R}^D} p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y}$$

for any  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 0$ . Let  $C_{S,1} = C_{S,1}(D, K, \tau_1)$  be the constant in Lemma 6. Since  $|p_{t_*}(\mathbf{x})| \leq C_{S,1}$  for any  $\mathbf{x} \in \mathbb{R}^D$ , we have

$$\begin{aligned} & \int_{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \geq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}} p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \\ & \leq C_{S,1} \int_{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \geq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} = C_{S,1} \mu_t^{-D} \int_{\|\mathbf{z}\|_\infty \geq \tau_{\text{tail}} \sqrt{\log(1/\delta)}} \phi_1(\mathbf{z}) d\mathbf{z} \\ & \leq C_{S,1} \mu_t^{-D} \sum_{i=1}^D \int_{|z_i| \geq \tau_{\text{tail}} \sqrt{\log(1/\delta)}} \phi(z_i) dz_i \leq 2C_{S,1} D \mu_t^{-D} \delta^{\frac{\tau_{\text{tail}}^2}{2}} \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 0$ , where the last inequality holds by the tail probability of the standard normal distribution. Also,

$$\begin{aligned} & \left| \int_{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \geq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}} \left( \frac{\mu_t y_i - x_i}{\sigma_t} \right) p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| \\ & \leq C_{S,1} \mu_t^{-D} \int_{\|\mathbf{z}\|_\infty \geq \tau_{\text{tail}} \sqrt{\log(1/\delta)}} |z_i| \phi_1(\mathbf{z}) d\mathbf{z} \leq C_{S,1} \mu_t^{-D} \sum_{j=1}^D \int_{|z_j| \geq \tau_{\text{tail}} \sqrt{\log(1/\delta)}} |z_j| \phi_1(\mathbf{z}) d\mathbf{z} \\ & = C_{S,1} \mu_t^{-D} \left\{ (D-1) \mathbb{E}[|Z|] \int_{|z| \geq \tau_{\text{tail}} \sqrt{\log(1/\delta)}} \phi(z) dz + \int_{|z| \geq \tau_{\text{tail}} \sqrt{\log(1/\delta)}} |z| \phi(z) dz \right\} \\ & \leq 2C_{S,1} \mu_t^{-D} \left\{ (D-1) \sqrt{2/\pi} \delta^{\tau_{\text{tail}}^2/2} + \sqrt{\mathbb{E}[Z^2]} \delta^{\tau_{\text{tail}}^2/4} \right\} \\ & \leq 2C_{S,1} D \mu_t^{-D} \delta^{\frac{\tau_{\text{tail}}^2}{4}}, \quad i \in [D] \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 0$ , where  $Z$  denotes the one-dimensional standard normal random variable and the second inequality holds by the Cauchy-Schwarz inequality. Note that  $\exp(-\bar{\tau}t) \leq \mu_t \leq \exp(-\underline{\tau}t)$  for  $t \geq 0$ . Then,

$$\begin{aligned} & \left| p_{t_*+t}(\mathbf{x}) - \int_{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}} p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| \leq 2C_{S,1} D \delta^{\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t}, \\ & \left\| \sigma_t \nabla p_{t_*+t}(\mathbf{x}) - \int_{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}} \left( \frac{\mu_t \mathbf{y} - \mathbf{x}}{\sigma_t} \right)^\top p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right\|_\infty \\ & \leq 2C_{S,1} D \delta^{\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t} \end{aligned} \tag{74}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 \leq t \leq \tau_t \log(1/\delta)$ . Lemma 6 implies that  $p_{t_*}(\mathbf{x}) \leq C_{S,1} \delta^{\tau_{\text{tail}}^2/2}$  for  $\|\mathbf{x}\|_\infty \geq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}$ . Then,

$$\begin{aligned} & \left| \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \geq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}}} p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| \\ & \leq 2C_{S,1} \delta^{\frac{\tau_{\text{tail}}^2}{2}} \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \geq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \\ & \leq C_{S,1} \mu_t^{-D} \delta^{\frac{\tau_{\text{tail}}^2}{2}} \int_{\mathbb{R}^D} \phi_1(\mathbf{z}) d\mathbf{z} \leq C_{S,1} \delta^{\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 \leq t \leq \tau_t \log(1/\delta)$ , where the last inequality holds because  $\mu_t^{-D} \leq \exp(D\bar{\tau}t)$ . Also,

$$\begin{aligned} & \left| \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \geq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}}} \left( \frac{\mu_t y_i - x_i}{\sigma_t} \right) p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| \\ & \leq C_{S,1} \delta^{\frac{\tau_{\text{tail}}^2}{2}} \mu_t^{-D} \int_{\mathbb{R}^D} |z_i| \phi_1(\mathbf{z}) d\mathbf{z} \leq \left( \sqrt{\frac{2}{\pi}} \right) C_{S,1} \delta^{\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 \leq t \leq \tau_t \log(1/\delta)$ . Combining with (74), we have

$$\begin{aligned} & \left| p_{t_*+t}(\mathbf{x}) - \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}}} p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| \\ & \leq C_{S,1} (2D + 1) \delta^{\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} \end{aligned} \quad (75)$$

and

$$\begin{aligned} & \left\| \sigma_t \nabla p_{t_*+t}(\mathbf{x}) - \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}}} \left( \frac{\mu_t \mathbf{y} - \mathbf{x}}{\sigma_t} \right)^\top p_{t_*}(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right\|_\infty \\ & \leq C_{S,1} (2D + \sqrt{2/\pi}) \delta^{\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t} \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 \leq t \leq \tau_t \log(1/\delta)$ . Let  $m_* \in \mathbb{N}_{\geq 2}$  be a large enough value as described below and  $\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(D_1)} \in \mathbb{R}^D$  be distinct vectors satisfying that

$$\left\{ \mathbf{y}^{(1)}, \dots, \mathbf{y}^{(D_1)} \right\} = \left\{ \tau_*(n_1, \dots, n_D)^\top : n_i \in \mathbb{Z}, i \in [D] \right\} \cap \left\{ \mathbf{y} \in \mathbb{R}^D : \|\mathbf{y}\|_\infty \leq (m_* - 1)\tau_* \right\},$$

where  $\tau_* = \{\mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}\} / m_*$  and  $D_1 = (2m_* - 1)^D$ . Let  $\mathcal{Y}_i = \{\mathbf{y} \in \mathbb{R}^D : \|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq \tau_*\}$  for  $i \in [D_1]$ . Taylor's theorem for multivariate function implies that

$$p_{t_*}(\mathbf{y}) = \sum_{0 \leq k < \tau_{\text{sm}}} \frac{(D^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} + \sum_{k := \tau_{\text{sm}}} \frac{(D^{\mathbf{k}} p_{t_*})(\xi \mathbf{y}^{(i)} + (1 - \xi)\mathbf{y})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}}$$

for a suitable  $\xi \in [0, 1]$  and  $i \in [D_1]$ ,  $\mathbf{y} \in \mathbb{R}^D$ , where  $(\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} = \prod_{j=1}^D (y_j - y_j^{(i)})^{k_j}$ ,  $\mathbf{k}! = \prod_{j=1}^D k_j!$  and  $k. = \|\mathbf{k}\|_1$ . Combining with Lemma 8, we have

$$\begin{aligned} & \left| p_{t_*}(\mathbf{y}) - \sum_{0 \leq k. < \tau_{\text{sm}}} \frac{(\mathbf{D}^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \right| \cdot 1\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_{\infty} \leq \tau_*\} \\ & \leq \sum_{k. = \tau_{\text{sm}}} C_{S,3} \sigma_{t_*}^{-\tau_{\text{sm}}} \prod_{j=1}^D \left( \frac{e\tau_*}{k_j} \right)^{k_j} \leq C_{S,3} (\tau_{\text{sm}} + 1)^D \left( \frac{e\tau_*}{\sigma_{t_*}} \right)^{\tau_{\text{sm}}} \end{aligned}$$

for  $\mathbf{y} \in \mathbb{R}^D$  and  $i \in [D_1]$  because  $k! \geq k^k e^{-k}$  for any  $k \in \mathbb{Z}_{\geq 0}$ , where  $C_{S,3} = C_{S,3}(D, K, \tau_{\text{sm}}, \bar{\tau}, \underline{\tau})$  is the constant in Lemma 8. Since  $\mathcal{Y}_1, \dots, \mathcal{Y}_{D_1}$  are mutually disjoint except on a set of Lebesgue measure zero and  $\bigcup_{i=1}^{D_1} \mathcal{Y}_i = \{\mathbf{y} \in \mathbb{R}^D : \|\mathbf{y}\|_{\infty} \leq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}\}$ , we have

$$\begin{aligned} & \int_{\|\mathbf{y}\|_{\infty} \leq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}} g(\mathbf{y}) d\mathbf{y} = \sum_{i=1}^{D_1} \int_{\|\mathbf{y} - \mathbf{y}^{(i)}\|_{\infty} \leq \tau_*} g(\mathbf{y}) d\mathbf{y} \\ & = \int_{\|\mathbf{y}\|_{\infty} \leq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}} \sum_{i=1}^{D_1} g(\mathbf{y}) \cdot 1\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_{\infty} \leq \tau_*\} d\mathbf{y} \end{aligned}$$

for any continuous function  $g : \mathbb{R}^D \rightarrow \mathbb{R}$ . Combining (75) with the last two displays, we have

$$\begin{aligned} & \left| p_{t_*+t}(\mathbf{x}) - \sum_{i=1}^{D_1} \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_{\infty} \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y} - \mathbf{y}^{(i)}\|_{\infty} \leq \tau_*}} \left\{ \sum_{0 \leq k. < \tau_{\text{sm}}} \frac{(\mathbf{D}^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)})}{\mathbf{k}!} (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \right\} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| \\ & \leq C_{S,1} (2D + 1) \delta^{\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} \\ & \quad + C_{S,3} (\tau_{\text{sm}} + 1)^D \left( \frac{e\tau_*}{\sigma_{t_*}} \right)^{\tau_{\text{sm}}} \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_{\infty} \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_{\infty} \leq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}} \sum_{i=1}^{D_1} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) \cdot 1\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_{\infty} \leq \tau_*\} d\mathbf{y} \\ & \leq C_{S,1} (2D + 1) \delta^{\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} + C_{S,3} (\tau_{\text{sm}} + 1)^D \left( \frac{e\tau_*}{\sigma_{t_*}} \right)^{\tau_{\text{sm}}} \delta^{-D\bar{\tau}\tau_t} \end{aligned} \tag{76}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 \leq t \leq \tau_t \log(1/\delta)$ , where the last inequality holds because  $\int_{\mathbb{R}^D} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} = \mu_t^{-D}$  and  $\mu_t^{-D} \leq \exp(D\bar{\tau}t) \leq \delta^{-D\bar{\tau}\tau_t}$ . Also, we have

$$\begin{aligned}
 & \left\| \sigma_t \nabla p_{t_*+t}(\mathbf{x}) - \sum_{i=1}^{D_1} \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq \tau_*}} \left\{ \sum_{0 \leq k < \tau_{\text{sm}}} \frac{(D^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)})}{\mathbf{k}!} \left( \frac{\mu_t \mathbf{y} - \mathbf{x}}{\sigma_t} \right)^\top (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \right\} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right\|_\infty \\
 & \leq C_{S,1} (2D + \sqrt{2/\pi}) \delta^{\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t} + C_{S,3} (\tau_{\text{sm}} + 1)^D \left( \frac{e\tau_*}{\sigma_{t_*}} \right)^{\tau_{\text{sm}}} \\
 & \quad \cdot \int_{\substack{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ \|\mathbf{y}\|_\infty \leq \mu_{t_*} + \tau_{\text{tail}} \sigma_{t_*} \sqrt{\log(1/\delta)}} \sum_{i=1}^{D_1} \left\| \frac{\mu_t \mathbf{y} - \mathbf{x}}{\sigma_t} \right\|_\infty \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) \cdot 1\{\|\mathbf{y} - \mathbf{y}^{(i)}\|_\infty \leq \tau_*\} d\mathbf{y} \\
 & \leq C_{S,1} (2D + \sqrt{2/\pi}) \delta^{\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t} + C_{S,3} \tau_{\text{tail}} (\tau_{\text{sm}} + 1)^D \left( \frac{e\tau_*}{\sigma_{t_*}} \right)^{\tau_{\text{sm}}} \delta^{-D\bar{\tau}\tau_t} \sqrt{\log(1/\delta)}
 \end{aligned} \tag{77}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 \leq t \leq \tau_t \log(1/\delta)$ , where the last inequality holds because  $\int_{\mathbb{R}^D} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} = \mu_t^{-D}$  and  $\mu_t^{-D} \leq \exp(D\bar{\tau}t) \leq \delta^{-D\bar{\tau}\tau_t}$ .

For  $x, y \in \mathbb{R}$  and  $t > 0$ , Taylor's theorem yields that

$$\left| \exp\left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right) - \sum_{l=0}^{D_2-1} \frac{1}{l!} \left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right)^l \right| \leq \frac{1}{D_2!} \left(\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right)^{D_2},$$

where  $D_2 = \lfloor 2e\tau_{\text{tail}}^2 \log(1/\delta) \rfloor + 1$  with small enough  $\delta$  so that  $D_2 \geq 1$ . For  $|x - \mu_t y| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)}$  and  $t \geq 0$ , the last display is further bounded by

$$\left( \frac{e\tau_{\text{tail}}^2 \log(1/\delta)}{D_2} \right)^{D_2} \leq 2^{-D_2} \leq \delta^{2e\tau_{\text{tail}}^2 \log 2} \leq \delta^{e\tau_{\text{tail}}^2},$$

where the last inequality holds because  $1/2 \leq \log 2$  and  $0 < \delta < 1$ . Then,

$$\begin{aligned}
 & \left| \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq \tau_*}} \left( \frac{\mu_t y - x}{\sigma_t} \right)^u (y - \tilde{y})^k \exp\left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right) dy \right. \\
 & \quad \left. - \sum_{l=0}^{D_2-1} \frac{1}{l!} \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq \tau_*}} \left( \frac{\mu_t y - x}{\sigma_t} \right)^u (y - \tilde{y})^k \left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right)^l dy \right| \\
 & \leq \delta^{e\tau_{\text{tail}}^2} \int_{\substack{|x - \mu_t y| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y - \tilde{y}| \leq \tau_*}} \left| \frac{\mu_t y - x}{\sigma_t} \right|^u |y - \tilde{y}|^k dy \\
 & \leq \delta^{e\tau_{\text{tail}}^2} \int_{|y| \leq m_* \tau_*} \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^u \tau_*^k dy = m_* \tau_*^{k+1} \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^u \delta^{e\tau_{\text{tail}}^2}
 \end{aligned}$$

for any  $x, \tilde{y} \in \mathbb{R}$  with  $|\tilde{y}| = (m_* - 1)\tau_*$ ,  $t \geq 0$ ,  $k \in \mathbb{Z}_{\geq 0}$  and  $u \in \{0, 1\}$ . Note that  $\mu_{t_*} \leq 1 - \tau_{t_*}/2 \leq 1$  and  $\sqrt{\tau_{t_*}} \leq \sigma_{t_*} \leq \sqrt{2\tau_{t_*}} \leq 1$  with  $t_* \leq (2\tau)^{-1}$ . For  $k \leq \tau_{\text{sm}}$ , the last display is bounded by

$$\begin{aligned} & (1 + \tau_{\text{tail}})^{k+1} m_*^{-k} \delta^{e\tau_{\text{tail}}^2} \{\log(1/\delta)\}^{\frac{k+1}{2}} \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^u \\ & \leq \tau_{\text{tail}} (1 + \tau_{\text{tail}})^{\tau_{\text{sm}}+1} \delta^{e\tau_{\text{tail}}^2} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}}{2}+1} \end{aligned}$$

because  $m_*\tau_* = \mu_{t_*} + \sigma_{t_*}\tau_{\text{tail}}\sqrt{\log(1/\delta)}$  and  $\mu_{t_*} + \sigma_{t_*}\tau_{\text{tail}}\sqrt{\log(1/\delta)} \leq (1 + \tau_{\text{tail}})\sqrt{\log(1/\delta)}$  with small enough  $\delta$  so that  $\delta \leq 1/e$  and  $\tau_{\text{tail}}\sqrt{\log(1/\delta)} \geq 1$ . Moreover,

$$\begin{aligned} & \left| \sum_{l=0}^{D_2-1} \frac{1}{l!} \int_{\substack{|x-\mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y-\tilde{y}| \leq \tau_*}} \left( \frac{\mu_t y - x}{\sigma_t} \right)^u (y - \tilde{y})^k \left( -\frac{(x - \mu_t y)^2}{2\sigma_t^2} \right)^l dy \right| \\ & \leq \tau_{\text{tail}} \left( 1 + \delta^{e\tau_{\text{tail}}^2} \right) (1 + \tau_{\text{tail}})^{\tau_{\text{sm}}+1} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}}{2}+1} \end{aligned}$$

for any  $x, \tilde{y} \in \mathbb{R}$  with  $|\tilde{y}| = (m_* - 1)\tau_*$ ,  $t \geq 0$ ,  $0 \leq k \leq \tau_{\text{sm}}$  and  $u \in \{0, 1\}$  because

$$\begin{aligned} & \left| \int_{\substack{|x-\mu_t y| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y-\tilde{y}| \leq \tau_*}} \left( \frac{\mu_t y - x}{\sigma_t} \right)^u (y - \tilde{y})^k \exp\left(-\frac{(x - \mu_t y)^2}{2\sigma_t^2}\right) dy \right| \\ & \leq \int_{|y| \leq m_*\tau_*} \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^u \tau_*^k dy \leq m_*\tau_*^{k+1} \tau_{\text{tail}} \sqrt{\log(1/\delta)} \\ & \leq \tau_{\text{tail}} (1 + \tau_{\text{tail}})^{\tau_{\text{sm}}+1} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}}{2}+1}. \end{aligned}$$

Note that  $|\prod_{j=1}^D x_j - \prod_{j=1}^D \tilde{x}_j| \leq DC^{D-1} \|\mathbf{x} - \tilde{\mathbf{x}}\|_{\infty}$  for any  $\mathbf{x}, \tilde{\mathbf{x}} \in [-C, C]^D$ . Since the last two displays are bounded by  $2\tau_{\text{tail}}(1 + \tau_{\text{tail}})^{\tau_{\text{sm}}+1} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}}{2}+1}$ , we have

$$\begin{aligned} & \left| \int_{\substack{\|\mathbf{x}-\mu_t \mathbf{y}\|_{\infty} \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ \|\mathbf{y}-\mathbf{y}^{(i)}\|_{\infty} \leq \tau_*}} \left( \frac{\mu_t y_h - x_h}{\sigma_t} \right)^u (\mathbf{y} - \mathbf{y}^{(i)})^{\mathbf{k}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} - \right. \\ & \left. \prod_{j=1}^D \sum_{l=0}^{D_2-1} \frac{1}{l! \sqrt{2\pi}\sigma_t} \int_{\substack{|x_j - \mu_t y_j| \leq \tau_{\text{tail}}\sigma_t\sqrt{\log(1/\delta)} \\ |y_j - y_j^{(i)}| \leq \tau_*}} \left( \frac{\mu_t y_h - x_h}{\sigma_t} \right)^{u \cdot 1_{\{h=j\}}} (y_j - y_j^{(i)})^{k_j} \left( -\frac{(x_j - \mu_t y_j)^2}{2\sigma_t^2} \right)^l dy_j \right| \\ & \leq (2\pi\sigma_t^2)^{-\frac{D}{2}} D 2^{D-1} \tau_{\text{tail}}^D (1 + \tau_{\text{tail}})^{D(\tau_{\text{sm}}+1)} \delta^{e\tau_{\text{tail}}^2} \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2}+1)} \end{aligned} \tag{78}$$

for  $\mathbf{x} \in \mathbb{R}^D$ ,  $t > 0$ ,  $h \in [D]$ ,  $i \in [D_1]$ ,  $j \in [D]$ ,  $\mathbf{k} \in \mathbb{Z}_{\geq 0}^D$  and  $u \in \{0, 1\}$  with  $k. \leq \tau_{\text{sm}}$ . With  $u = 0$  in the last display, the second integral satisfies that

$$\begin{aligned}
 & \frac{1}{l! \sqrt{2\pi} \sigma_t} \int_{\substack{|x_j - \mu_t y_j| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y_j - y_j^{(i)}| \leq \tau_*}} (y_j - y_j^{(i)})^{k_j} \left( -\frac{(x_j - \mu_t y_j)^2}{2\sigma_t^2} \right)^l dy_j \\
 &= \frac{\mu_t^{-1}}{l! \sqrt{2\pi}} \int_{\substack{|z_j| \leq \tau_{\text{tail}} \sqrt{\log(1/\delta)} \\ |\mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)}| \leq \tau_*}} \left( \mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)} \right)^{k_j} z_j^{2l} (-2)^{-l} dz_j \\
 &= \frac{(-2)^{-l} \mu_t^{-1}}{l! \sqrt{2\pi}} \int_{\substack{|z_j| \leq \tau_{\text{tail}} \sqrt{\log(1/\delta)} \\ |\mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)}| \leq \tau_*}} \sum_{r_j=0}^{k_j} \binom{k_j}{r_j} (\mu_t^{-1} \sigma_t)^{r_j} \left( \mu_t^{-1} x_j - y_j^{(i)} \right)^{k_j - r_j} z_j^{r_j + 2l} dz_j \\
 &= \frac{(-2)^{-l} \mu_t^{-k_j - 1}}{l! \sqrt{2\pi}} \sum_{r_j=0}^{k_j} \binom{k_j}{r_j} \sigma_t^{r_j} \left( x_j - \mu_t y_j^{(i)} \right)^{k_j - r_j} \left( \frac{\bar{z}_{i,j}^{r_j + 2l + 1} - \underline{z}_{i,j}^{r_j + 2l + 1}}{r_j + 2l + 1} \right) \stackrel{\text{def}}{=} P_{i,j,k_j,l}(x_j, t),
 \end{aligned}$$

where

$$\begin{aligned}
 \bar{z}_{i,j} &= \min \left( \max \left( \frac{\mu_t(y_j^{(i)} + \tau_*) - x_j}{\sigma_t}, -\tau_{\text{tail}} \sqrt{\log(1/\delta)} \right), \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right), \\
 \underline{z}_{i,j} &= \min \left( \max \left( \frac{\mu_t(y_j^{(i)} - \tau_*) - x_j}{\sigma_t}, -\tau_{\text{tail}} \sqrt{\log(1/\delta)} \right), \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right).
 \end{aligned}$$

Combining (76) and (78) with the last two displays, we have

$$\begin{aligned}
 & |p_{t_*+t}(\mathbf{x}) - g_{t_*,t}(\mathbf{x})| \\
 & \leq C_{S,1} (2D+1) \delta^{\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} + C_{S,3} (\tau_{\text{sm}} + 1)^D \left( \frac{e\tau_*}{\sigma_{t_*}} \right)^{\tau_{\text{sm}}} \delta^{-D\bar{\tau}\tau_t} \\
 & \quad + \sum_{i=1}^{D_1} \sum_{0 \leq k. < \tau_{\text{sm}}} \left| \frac{(\mathbf{D}^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)})}{\mathbf{k}!} \right| (2\pi\sigma_t^2)^{-\frac{D}{2}} D 2^{D-1} \tau_{\text{tail}}^D (1 + \tau_{\text{tail}})^{D(\tau_{\text{sm}}+1)} \delta e \tau_{\text{tail}}^2 \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2}+1)}
 \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $0 < t \leq \tau_t \log(1/\delta)$ , where  $g_{t_*,t} : \mathbb{R}^D \rightarrow \mathbb{R}$  is a function such that

$$g_{t_*,t}(\mathbf{x}) = \sum_{i=1}^{D_1} \sum_{0 \leq k. < \tau_{\text{sm}}} \left\{ \frac{(\mathbf{D}^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)})}{\mathbf{k}!} \right\} \prod_{j=1}^D \sum_{l=0}^{D_2-1} P_{i,j,k_j,l}(x_j, t)$$

for  $\mathbf{x} \in \mathbb{R}^D$ . Let

$$m_* = \lfloor m^{1/D} + 1 \rfloor \quad \text{and} \quad t_* = m^{-\frac{2-2\tau_{\text{low}}}{D}}$$

with large enough  $m \in \mathbb{R}$  so that  $t_* \leq (2\bar{\tau})^{-1}$  and  $m_* \in \mathbb{N}_{\geq 2}$ . Since  $\sigma_t^2 \geq 1 - \exp(-2\bar{\tau}t)$  for  $t \geq 0$  and  $1 - \exp(-x) \geq x/2$  for  $0 \leq x \leq 1$ , we have  $\sigma_t^{-D} \leq (\bar{\tau}\delta)^{-D/2}$  for  $t \geq \delta$  with

$\delta \leq \underline{\tau}^{-1}$ . Then,

$$\begin{aligned} & |p_{t_*+t}(\mathbf{x}) - g_{t_*,t}(\mathbf{x})| \\ & \leq D_3 \left[ \delta^{\frac{D\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} + m_*^{-\tau_{\text{sm}}} t_*^{-\frac{\tau_{\text{sm}}}{2}} \delta^{-D\bar{\tau}\tau_t} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}}{2}} + m_*^D t_*^{-\frac{\tau_{\text{sm}}}{2}} \delta e^{\tau_{\text{tail}}^2 - D} \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2} + 1)} \right] \\ & \leq D_3 \left[ \delta^{\frac{D\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t} + m^{-\frac{\tau_{\text{low}}\tau_{\text{sm}}}{D}} \delta^{-D\bar{\tau}\tau_t} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}}{2}} + 2^D m^{\frac{D+1-\tau_{\text{low}}}{D}} \delta e^{\tau_{\text{tail}}^2 - D} \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2} + 1)} \right] \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ , where  $D_3 = D_3(D, \tau_{\text{sm}}, \underline{\tau}, \tau_{\text{tail}}, C_{S,1}, C_{S,3})$  and the last inequality holds because  $m^{1/D} \leq m_* \leq 2m^{1/D}$ . Since  $\tau_{\text{tail}}^2 = 4(D\bar{\tau}\tau_t + 1) \vee (D+1)/e$ , we have

$$\frac{\tau_{\text{tail}}^2}{2} - D\bar{\tau}\tau_t \geq 1 \quad \text{and} \quad e^{\tau_{\text{tail}}^2 - D} \geq 1.$$

Then,

$$\begin{aligned} & |p_{t_*+t}(\mathbf{x}) - g_{t_*,t}(\mathbf{x})| \\ & \leq D_3 \left[ \delta + m^{-\frac{\tau_{\text{low}}\tau_{\text{sm}}}{D}} \delta^{-D\bar{\tau}\tau_t} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}}{2}} + 2^D m^{\frac{D+1-\tau_{\text{low}}}{D}} \delta \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2} + 1)} \right] \end{aligned} \quad (79)$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ . Similarly, with  $u = 1$  and  $h = j$  in (78), the last integral in (78) satisfies that

$$\begin{aligned} & \frac{1}{l! \sqrt{2\pi}\sigma_t} \int_{\substack{|x_j - \mu_t y_j| \leq \tau_{\text{tail}} \sigma_t \sqrt{\log(1/\delta)} \\ |y_j - y_j^{(i)}| \leq \tau_*}} \left( \frac{\mu_t y_j - x_j}{\sigma_t} \right) (y_j - y_j^{(i)})^{k_j} \left( -\frac{(x_j - \mu_t y_j)^2}{2\sigma_t^2} \right)^l dy_j \\ & = \frac{\mu_t^{-1}}{l! \sqrt{2\pi}} \int_{\substack{|z_j| \leq \tau_{\text{tail}} \sqrt{\log(1/\delta)} \\ |\mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)}| \leq \tilde{\tau}_*}} \left( \mu_t^{-1} \sigma_t z_j + \mu_t^{-1} x_j - y_j^{(i)} \right)^{k_j} z_j^{2l+1} (-2)^{-l} dz_j \\ & = \frac{(-2)^{-l} \mu_t^{-k_j-1}}{l! \sqrt{2\pi}} \sum_{r_j=0}^{k_j} \binom{k_j}{r_j} \sigma_t^{r_j} \left( x_j - \mu_t y_j^{(i)} \right)^{k_j - r_j} \left( \frac{\tilde{z}_{i,j}^{r_j+2l+2} - \underline{\tilde{z}}_{i,j}^{r_j+2l+2}}{r_j + 2l + 2} \right) \stackrel{\text{def}}{=} \tilde{P}_{i,j,k_j,l}(x_j, t). \end{aligned}$$

Combining (77) and (78) with the last display, we have

$$\begin{aligned} & \left| \sigma_t (\nabla p_{t_*+t}(\mathbf{x}))_h - \tilde{g}_{t_*,t}^{(h)}(\mathbf{x}) \right| \\ & \leq C_{S,1} (2D + \sqrt{2/\pi}) \delta^{\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t} + C_{S,3} \tau_{\text{tail}} (\tau_{\text{sm}} + 1)^D \left( \frac{e\tau_*}{\sigma_{t_*}} \right)^{\tau_{\text{sm}}} \delta^{-D\bar{\tau}\tau_t} \sqrt{\log(1/\delta)} \\ & \quad + \sum_{i=1}^{D_1} \sum_{0 \leq k. < \tau_{\text{sm}}} \left| \frac{(\mathbf{D}^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)})}{\mathbf{k}!} \right| (2\pi\sigma_t^2)^{-\frac{D}{2}} D 2^{D-1} \tau_{\text{tail}}^D (1 + \tau_{\text{tail}})^{D(\tau_{\text{sm}}+1)} \delta e^{\tau_{\text{tail}}^2} \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2} + 1)} \\ & \leq D_4 \left[ \delta^{\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t} + m_*^{-\tau_{\text{sm}}} t_*^{-\frac{\tau_{\text{sm}}}{2}} \delta^{-D\bar{\tau}\tau_t} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}+1}{2}} + m_*^D t_*^{-\frac{\tau_{\text{sm}}}{2}} \delta e^{\tau_{\text{tail}}^2 - D} \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2} + 1)} \right] \\ & = D_4 \left[ \delta^{\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t} + m^{-\frac{\tau_{\text{low}}\tau_{\text{sm}}}{D}} \delta^{-D\bar{\tau}\tau_t} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}+1}{2}} + 2^D m^{\frac{D+1-\tau_{\text{low}}}{D}} \delta e^{\tau_{\text{tail}}^2 - D} \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2} + 1)} \right] \end{aligned}$$

for  $h \in [D]$ ,  $\mathbf{x} \in \mathbb{R}^D$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ , where  $D_4 = D_4(D, \tau_{\text{sm}}, \mathcal{I}, \tau_{\text{tail}}, C_{S,1}, C_{S,3})$  and  $\tilde{g}_{t_*,t}^{(h)} : \mathbb{R}^D \rightarrow \mathbb{R}$ ,  $h \in [D]$  is a function such that

$$\tilde{g}_{t_*,t}^{(h)}(\mathbf{x}) = \sum_{i=1}^{D_1} \sum_{0 \leq k < \tau_{\text{sm}}} \left\{ (D^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)}) \right\} \left\{ \prod_{\substack{j=1 \\ j \neq h}}^D \sum_{l=0}^{D_2-1} \frac{P_{i,j,k_j,l}(x_j, t)}{k_j!} \right\} \left\{ \sum_{l=0}^{D_2-1} \frac{\tilde{P}_{i,h,k_h,l}(x_h, t)}{k_h!} \right\}.$$

Since  $\tau_{\text{tail}}^2 = 4(D\bar{\tau}\tau_t + 1) \vee (D+1)/e$ , we have

$$\frac{\tau_{\text{tail}}^2}{4} - D\bar{\tau}\tau_t \geq 1 \quad \text{and} \quad e\tau_{\text{tail}}^2 - D \geq 1.$$

Then,

$$\begin{aligned} & \left| \sigma_t (\nabla p_{t_*+t}(\mathbf{x}))_h - \tilde{g}_{t_*,t}^{(h)}(\mathbf{x}) \right| \\ & \leq D_4 \left[ \delta + m^{-\frac{\tau_{\text{low}}\tau_{\text{sm}}}{D}} \delta^{-D\bar{\tau}\tau_t} \{\log(1/\delta)\}^{\frac{\tau_{\text{sm}}+1}{2}} + 2^D m^{\frac{D+1-\tau_{\text{low}}}{D}} \delta \{\log(1/\delta)\}^{D(\frac{\tau_{\text{sm}}}{2}+1)} \right], \quad h \in [D] \end{aligned} \quad (80)$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ . Let

$$\delta = m^{-\frac{\tau_{\text{low}}\tau_{\text{sm}}+D+1-\tau_{\text{low}}}{D(1+D\bar{\tau}\tau_t)}}$$

for large enough  $m \in \mathbb{R}$ . Combining (79) and (80) with the last display, we have

$$\begin{aligned} |p_{t_*+t}(\mathbf{x}) - g_{t_*,t}(\mathbf{x})| & \leq D_5 m^{-\frac{\tau_{\text{low}}\tau_{\text{sm}}-(D+1-\tau_{\text{low}})D\bar{\tau}\tau_t}{D(1+D\bar{\tau}\tau_t)}} (\log m)^{D(\frac{\tau_{\text{sm}}}{2}+1)}, \\ \left| \sigma_t (\nabla p_{t_*+t}(\mathbf{x}))_h - \tilde{g}_{t_*,t}^{(h)}(\mathbf{x}) \right| & \leq D_5 m^{-\frac{\tau_{\text{low}}\tau_{\text{sm}}-(D+1-\tau_{\text{low}})D\bar{\tau}\tau_t}{D(1+D\bar{\tau}\tau_t)}} (\log m)^{D(\frac{\tau_{\text{sm}}}{2}+1)}, \quad h \in [D] \end{aligned} \quad (81)$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ , where  $D_5 = D_5(D, \bar{\tau}, \tau_t, \tau_{\text{sm}}, \tau_{\text{low}}, D_3, D_4)$ .

Let  $0 < \tilde{\delta} < \delta$  be a small enough value as described below. With  $\tilde{\delta}^2 < 1/2$ , Lemma 18 implies that there exist neural networks  $f_\mu \in \mathcal{F}_{\text{NN}}(L_\mu, \mathbf{d}_\mu, s_\mu, M_\mu)$ ,  $f_\sigma \in \mathcal{F}_{\text{NN}}(L_\sigma, \mathbf{d}_\sigma, s_\sigma, M_\sigma)$  with

$$\begin{aligned} L_\mu, L_\sigma & \leq C_{N,4} \{\log(1/\tilde{\delta})\}^2, \quad \|\mathbf{d}_\mu\|_\infty, \|\mathbf{d}_\sigma\|_\infty \leq C_{N,4} \{\log(1/\tilde{\delta})\}^2 \\ s_\mu, s_\sigma & \leq C_{N,4} \{\log(1/\tilde{\delta})\}^3, \quad M_\mu, M_\sigma \leq C_{N,4} \log(1/\tilde{\delta}) \end{aligned} \quad (82)$$

such that  $|\mu_t - f_\mu(t)| \leq \tilde{\delta}$  for  $t \geq 0$  and  $|\sigma_t - f_\sigma(t)| \leq \tilde{\delta}$  for  $t \geq \tilde{\delta}$ , where  $C_{N,4}$  is the constant in Lemma 18. Also, Lemma 19 implies that there exist a neural network  $f_{\text{rec}} \in \mathcal{F}_{\text{NN}}(L_{\text{rec}}, \mathbf{d}_{\text{rec}}, s_{\text{rec}}, M_{\text{rec}})$  with

$$\begin{aligned} L_{\text{rec}} & \leq C_{N,5} \{\log(1/\tilde{\delta})\}^2, \quad \|\mathbf{d}_{\text{rec}}\|_\infty \leq C_{N,5} \{\log(1/\tilde{\delta})\}^3 \\ s_{\text{rec}} & \leq C_{N,5} \{\log(1/\tilde{\delta})\}^4, \quad M_{\text{rec}} \leq C_{N,5} \tilde{\delta}^{-2} \end{aligned}$$

such that  $|1/x - f_{\text{rec}}(x)| \leq \tilde{\delta}$  for any  $x \in [\tilde{\delta}, 1/\tilde{\delta}]$ , where  $C_{N,5}$  is the constant in Lemma 19. Since  $\sigma_t - \tilde{\delta} \leq f_\sigma(t) \leq \sigma_t + \tilde{\delta}$  for  $t \geq \tilde{\delta}$  and  $\sqrt{\tau\tilde{\delta}} \leq \sigma_t \leq 1$  for  $t \geq \delta$ , we have  $\delta \leq f_\sigma(t) \leq 2$  for  $t \geq \delta$  with small enough  $\tilde{\delta}$  so that  $\tilde{\delta} \leq \sqrt{\tau\tilde{\delta}} - \delta$  and  $\tilde{\delta} \leq 1$ . Then,

$$\begin{aligned} |1/\sigma_t - f_{\text{rec}}(f_\sigma(t))| &\leq |1/\sigma_t - 1/f_\sigma(t)| + |1/f_\sigma(t) - f_{\text{rec}}(f_\sigma(t))| \\ &\leq \{\sigma_t \wedge f_\sigma(t)\}^{-2} |\sigma_t - f_\sigma(t)| + \tilde{\delta} \leq (1 + \delta^{-2})\tilde{\delta} \end{aligned} \quad (83)$$

for  $t \geq \delta$ . Since  $\mu_t - \tilde{\delta} \leq f_\mu(t) \leq \mu_t + \tilde{\delta}$  for  $t \geq \tilde{\delta}$  and  $\delta^{\bar{\tau}\tau_t} \leq \mu_t \leq 1$  for  $0 \leq t \leq \tau_t \log(1/\delta)$ , we have  $\delta^{\bar{\tau}\tau_t}/2 \leq f_\mu(t) \leq 2$  for  $\delta \leq t \leq \tau_t \log(1/\delta)$  with small enough  $\tilde{\delta}$  so that  $\tilde{\delta} \leq \delta^{\bar{\tau}\tau_t}/2$  and  $\tilde{\delta} \leq 1$ . Then,

$$\begin{aligned} |1/\mu_t - f_{\text{rec}}(f_\mu(t))| &\leq |1/\mu_t - 1/f_\mu(t)| + |1/f_\mu(t) - f_{\text{rec}}(f_\mu(t))| \\ &\leq \{\mu_t \wedge f_\mu(t)\}^{-2} |\mu_t - f_\mu(t)| + \tilde{\delta} \leq (1 + 4\delta^{-2\bar{\tau}\tau_t})\tilde{\delta} \end{aligned} \quad (84)$$

for  $\delta \leq t \leq \tau_t \log(1/\delta)$ . Lemma 14 implies that for  $k \geq 2$ , there exists a neural network  $\tilde{f}_{\text{mult}}^{(k)} \in \mathcal{F}_{\text{NN}}(\tilde{L}_{\text{mult}}^{(k)}, \tilde{\mathbf{d}}_{\text{mult}}^{(k)}, \tilde{s}_{\text{mult}}^{(k)}, \tilde{M}_{\text{mult}}^{(k)})$  with

$$\begin{aligned} \tilde{L}_{\text{mult}}^{(k)} &\leq C_{N,1} \log k \{\log(1/\tilde{\delta}) + \bar{\tau}\tau_t \log(1/\delta)\}, \quad \tilde{\mathbf{d}}_{\text{mult}}^{(k)} = (k, 48k, \dots, 48k, 1)^\top, \\ \tilde{s}_{\text{mult}}^{(2)} &\leq C_{N,1} k \{\log(1/\tilde{\delta}) + \bar{\tau}\tau_t \log(1/\delta)\}, \quad \tilde{M}_{\text{mult}}^{(k)} = \delta^{-\bar{\tau}\tau_t k} \end{aligned}$$

such that

$$\left| \tilde{f}_{\text{mult}}^{(k)}(\tilde{x}_1, \dots, \tilde{x}_k) - \prod_{i=1}^k x_i \right| \leq \tilde{\delta} + k\delta^{-\bar{\tau}\tau_t(k-1)}\tilde{\epsilon} \quad (85)$$

for any  $\mathbf{x} = (x_1, \dots, x_k) \in \mathbb{R}^k$  with  $\|\mathbf{x}\|_\infty \leq \delta^{-1}$  and  $\tilde{\mathbf{x}} = (\tilde{x}_1, \dots, \tilde{x}_k) \in \mathbb{R}^k$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ , where  $0 < \tilde{\epsilon} \leq 1$  and  $C_{N,1}$  is the constant in Lemma 14. Let

$$f_{\text{clip}} \in \mathcal{F}_{\text{NN}}(2, (1, 2, 1)^\top, 7, \tau_{\text{tail}}\sqrt{\log(1/\delta)})$$

be the neural network in Lemma 15 such that  $f_{\text{clip}}(x) = (x \vee -\tau_{\text{tail}}\sqrt{\log(1/\delta)}) \wedge \tau_{\text{tail}}\sqrt{\log(1/\delta)}$  for  $x \in \mathbb{R}$ . For  $i \in [D_1]$  and  $j \in [D]$ , consider functions  $\bar{f}_{i,j}, \underline{f}_{i,j} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} \bar{f}_{i,j}(x, t) &= f_{\text{clip}}\left(\tilde{f}_{\text{mult}}^{(2)}\left(f_{\text{rec}}(f_\sigma(t)), \{y_j^{(i)} + \tau_*\}f_\mu(t) - x\right)\right), \\ \underline{f}_{i,j}(x, t) &= f_{\text{clip}}\left(\tilde{f}_{\text{mult}}^{(2)}\left(f_{\text{rec}}(f_\sigma(t)), \{y_j^{(i)} - \tau_*\}f_\mu(t) - x\right)\right), \end{aligned}$$

for  $x, t \in \mathbb{R}$ . Note that both  $|y_j^{(i)} + \tau_*|$  and  $|y_j^{(i)} - \tau_*|$  are upper bounded by  $m_*\tau_* \leq (1 + \tau_{\text{tail}})\sqrt{\log(1/\delta)}$ . Then, for  $|x| \leq 1 + \tau_x\sqrt{\log(1/\delta)}$ , both  $|(y_j^{(i)} + \tau_*)\mu_t - x|$  and  $|(y_j^{(i)} - \tau_*)\mu_t - x|$  are upper bounded by  $\delta^{-\bar{\tau}\tau_t}$  with small enough  $\delta$ . Combining (82), (83) and (85) with the last display, both  $|\bar{z}_{i,j} - \bar{f}_{i,j}(x, t)|$  and  $|\underline{z}_{i,j} - \underline{f}_{i,j}(x, t)|$  are bounded by

$$\tilde{\delta} + 2\delta^{-\bar{\tau}\tau_t}(1 + \delta^{-2\bar{\tau}\tau_t}/4)\tilde{\delta} \leq 5\delta^{-3\bar{\tau}\tau_t}\tilde{\delta}, \quad (86)$$

for  $|x| \leq \mu_t + \tau_x\sigma_t\sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ . Since  $\mu_t - \tilde{\delta} \leq f_\mu(t) \leq \mu_t + \tilde{\delta}$  for  $t \geq \tilde{\delta}$ , we have  $1/4 \leq 1/2 - \tilde{\delta} \leq f_\mu(t) \leq 1 + \tilde{\delta} \leq 2$  and  $1/4 \leq \mu_t \leq 2$  for  $\delta \leq t \leq D_1$  with

small enough  $\tilde{\delta}$  by (27). For any  $i \in [D_2], j \in [D], k \in \{0, \dots, \tau_{\text{sm}} - 1\}$ , consider functions  $f_{i,j,k}, \tilde{f}_{i,j,k} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} f_{i,j,k}(x, t) &= \sum_{l=0}^{D_2-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{(-2)^{-l}}{k!l!\sqrt{2\pi}(r+2l+1)} \right\} \left\{ \bar{f}_{i,j,k,l,r,r+2l+1} - \underline{f}_{i,j,k,l,r,r+2l+1} \right\}, \\ \tilde{f}_{i,j,k}(x, t) &= \sum_{l=0}^{D_2-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{(-2)^{-l}}{k!l!\sqrt{2\pi}(r+2l+2)} \right\} \left\{ \bar{f}_{i,j,k,l,r,r+2l+2} - \underline{f}_{i,j,k,l,r,r+2l+2} \right\}, \end{aligned}$$

for  $x, t \in \mathbb{R}$ , where

$$\begin{aligned} \bar{f}_{i,j,k,l,r,s} &= \tilde{f}_{\text{mult}}^{(2k+s+1)} \left( f_{\text{rec}}(f_\mu(t)) \cdot \mathbf{1}_{k+1}, f_\sigma(t) \cdot \mathbf{1}_r, \left\{ x - y_j^{(i)} f_\mu(t) \right\} \cdot \mathbf{1}_{k-r}, \bar{f}_{i,j}(x, t) \cdot \mathbf{1}_s \right), \\ \underline{f}_{i,j,k,l,r,s} &= \tilde{f}_{\text{mult}}^{(2k+s+1)} \left( f_{\text{rec}}(f_\mu(t)) \cdot \mathbf{1}_{k+1}, f_\sigma(t) \cdot \mathbf{1}_r, \left\{ x - y_j^{(i)} f_\mu(t) \right\} \cdot \mathbf{1}_{k-r}, \underline{f}_{i,j}(x, t) \cdot \mathbf{1}_s \right), \end{aligned}$$

for  $s \in \{r+2l+1, r+2l+2\}$ . Combining (82), (84), (86) and (85) with the last two displays, we have

$$\begin{aligned} & \left| \sum_{l=0}^{D_2-1} \frac{P_{i,j,k,l}(x, t)}{k!} - f_{i,j,k}(x, t) \right| \\ & \leq \sum_{l=0}^{D_2-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{2^{-l+1}}{k!l!\sqrt{2\pi}(2r+r+2l+1)} \right\} \left\{ \tilde{\delta} + 5(2k+r+2l+2)\delta^{-(2k+r+2l+4)\bar{\tau}\tau_t} \tilde{\delta} \right\} \end{aligned}$$

and

$$\begin{aligned} & \left| \sum_{l=0}^{D_2-1} \frac{P_{i,j,k,l}(x, t)}{k!} - f_{i,j,k}(x, t) \right| \\ & \leq \sum_{l=0}^{D_2-1} \sum_{r=0}^k \binom{k}{r} \left\{ \frac{2^{-l+1}}{k!l!\sqrt{2\pi}(r+2l+2)} \right\} \left\{ \tilde{\delta} + 5(2k+r+2l+3)\delta^{-(2k+r+2l+5)\bar{\tau}\tau_t} \tilde{\delta} \right\} \end{aligned}$$

for  $i \in [D_1], j \in [D], k \in \{0, \dots, \tau_{\text{sm}} - 1\}, |x| \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$  with small enough  $\delta$  so that  $\sigma_t, |x - \mu_t y_j^{(i)}|, \tau_{\text{tail}} \sqrt{\log(1/\delta)}$  are bounded by  $\delta^{-\bar{\tau}\tau_t}$ . Since  $\sum_{r=0}^k \binom{k}{r} = 2^k$  and  $2^k/k! \leq 2$  for all  $k \in \mathbb{N}$ , the last two displays are bounded by

$$\sum_{l=0}^{D_2-1} \left( \frac{2^{-l+2}}{l!\sqrt{2\pi}(2l+1)} \right) \left\{ 1 + 5(3\tau_{\text{sm}} + 2l)\delta^{-(3\tau_{\text{sm}}+2l+1)\bar{\tau}\tau_t} \right\} \tilde{\delta} \leq \delta^{-D_6 \log(1/\delta)} \tilde{\delta}, \quad (87)$$

where  $D_6 = D_6(\bar{\tau}, \tau_{\text{tail}}, \tau_{\text{sm}}, \tau_t)$ . For any  $i \in [D_1], j \in [D], k \in \{0, \dots, \tau_{\text{sm}} - 1\}, l \in \{0, \dots, D_2 - 1\}, |x| \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ , we have

$$\begin{aligned} & \left| \frac{P_{i,j,k,l}(x, t)}{k!} \right| \\ & \leq \left\{ \frac{2^{-l+1} \mu_t^{-k-1}}{k!l!\sqrt{2\pi}(r+2l+1)} \sum_{r=0}^k \binom{k}{r} \right\} \left\{ (2 + \tau_x + \tau_{\text{tail}}) \sqrt{\log(1/\delta)} \right\}^k \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^{k+2l+1} \end{aligned}$$

and

$$\begin{aligned} & \left| \frac{\tilde{P}_{i,j,k,l}(x,t)}{k!} \right| \\ & \leq \left\{ \frac{2^{-l+1} \mu_t^{-k-1}}{k! l! \sqrt{2\pi} (r+2l+2)} \sum_{r=0}^k \binom{k}{r} \right\} \left\{ (2 + \tau_x + \tau_{\text{tail}}) \sqrt{\log(1/\delta)} \right\}^k \left\{ \tau_{\text{tail}} \sqrt{\log(1/\delta)} \right\}^{k+2l+2} \end{aligned}$$

because  $\mu_t \leq 1, \sigma_t \leq 1$ , and  $y_j^{(i)} \leq m_* \tau_* \leq (1 + \tau_{\text{tail}}) \sqrt{\log(1/\delta)}$ . Since  $\sum_{r=0}^k \binom{k}{r} = 2^k$  and  $2^k/k! \leq 2$  for all  $k \in \mathbb{N}$ , the last two displays are bounded by

$$\left( \frac{4}{\sqrt{2\pi}} \right) \delta^{-k\bar{\tau}\tau_t} \left\{ (2 + \tau_x + \tau_{\text{tail}})^2 \tau_{\text{tail}}^2 \log(1/\delta) \right\}^{k+l+1}.$$

Then, both  $|\sum_{l=0}^{D_2-1} P_{i,j,k,l}(x,t)/k!|$  and  $|\sum_{l=0}^{D_2-1} \tilde{P}_{i,j,k,l}(x,t)/k!|$  are upper bounded by

$$D_2 \left( \frac{4}{\sqrt{2\pi}} \right) \delta^{-(\tau_{\text{sm}}-1)\bar{\tau}\tau_t} \left\{ (2 + \tau_x + \tau_{\text{tail}})^2 \tau_{\text{tail}}^2 \log(1/\delta) \right\}^{\tau_{\text{sm}}+D_2-1} \leq \{\log(1/\delta)\}^{D_7 \log(1/\delta)}$$

for  $i \in [D_1], j \in [D], k \in \{0, \dots, \tau_{\text{sm}} - 1\}, |x| \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ , where  $D_7 = D_7(\tau_{\text{tail}}, \tau_{\text{sm}}, \tau_x, \tau_t, \bar{\tau})$ . Consider functions  $f_{t_*}, \tilde{f}_{t_*}^{(1)}, \dots, \tilde{f}_{t_*}^{(D)} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} f_{t_*}(\mathbf{x}, t) &= \sum_{i=1}^{D_1} \sum_{0 \leq k < \tau_{\text{sm}}} \left\{ (D^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)}) \right\} f_{\text{mult}}^{(D)}(f_{i,1,k_1}(x_1, t), \dots, f_{i,D,k_D}(x_D, t)) \quad \text{and} \\ \tilde{f}_{t_*}^{(h)}(\mathbf{x}, t) &= \sum_{i=1}^{D_1} \sum_{0 \leq k < \tau_{\text{sm}}} \left\{ (D^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)}) \right\} f_{\text{mult}}^{(D)} \left( \tilde{f}_{i,h,k_h}(x_h, t), \underbrace{f_{i,1,k_1}(x_1, t), \dots, f_{i,D,k_D}(x_D, t)}_{\text{without } f_{i,h,k_h}(x_h, t)} \right), \end{aligned}$$

where  $f_{\text{mult}}^{(D)} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}^{(D)}, \mathbf{d}_{\text{mult}}^{(D)}, s_{\text{mult}}^{(D)}, M_{\text{mult}}^{(D)})$  is the neural network in Lemma 14 with

$$\begin{aligned} L_{\text{mult}}^{(D)} &\leq C_{N,1} \log D [\log(1/\delta) + DD_7 \log(1/\delta) \log \log(1/\delta)], \quad \mathbf{d}_{\text{mult}}^{(D)} = (D, 48D, \dots, 48D, 1)^\top, \\ s_{\text{mult}}^{(D)} &\leq C_{N,1} D [\log(1/\delta) + D_7 \log(1/\delta) \log \log(1/\delta)], \quad M_{\text{mult}}^{(D)} = \{\log(1/\delta)\}^{DD_7 \log(1/\delta)} \end{aligned}$$

such that

$$\left| \tilde{f}_{\text{mult}}^{(D)}(\tilde{x}_1, \dots, \tilde{x}_D) - \prod_{i=1}^D x_i \right| \leq \tilde{\delta} + D \{\log(1/\delta)\}^{(D-1)D_7 \log(1/\delta)} \tilde{\epsilon}$$

for any  $\mathbf{x} = (x_1, \dots, x_D) \in \mathbb{R}^D$  with  $\|\mathbf{x}\|_\infty \leq \{\log(1/\delta)\}^{DD_7 \log(1/\delta)}$  and  $\tilde{\mathbf{x}} = (\tilde{x}_1, \dots, \tilde{x}_D) \in \mathbb{R}^D$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ . Combining (87) with the last display, we have

$$\begin{aligned} & |f_{t_*}(\mathbf{x}, t) - g_t(\mathbf{x})| \\ & \leq \sum_{i=1}^{D_1} \sum_{0 \leq k < \tau_{\text{sm}}} \left| (D^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)}) \right| \left\{ 1 + D \delta^{-D_6 \log(1/\delta)} \{\log(1/\delta)\}^{(D-1)D_7 \log(1/\delta)} \right\} \tilde{\delta} \\ & \leq D_1 \tau_{\text{sm}}^D C_{S,3} \sigma_{t_*}^{-\tau_{\text{sm}}} \left\{ 1 + D \delta^{-D_6 \log(1/\delta)} \{\log(1/\delta)\}^{(D-1)D_7 \log(1/\delta)} \right\} \tilde{\delta} \\ & \leq m \frac{\tau_{\text{sm}}(1-\tau_{\text{low}})+D}{D} \delta^{-D_8 \log(1/\delta)} \tilde{\delta} \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ , where  $D_8 = D_8(D, \underline{\tau}, \tau_{\text{sm}}, C_{S,3}, D_6, D_7)$ . Similarly, we have

$$\begin{aligned} & \left| \tilde{f}_{t_*}^{(h)}(\mathbf{x}, t) - \tilde{g}_t^{(h)}(\mathbf{x}) \right| \\ & \leq \sum_{i=1}^{D_1} \sum_{0 \leq k < \tau_{\text{sm}}} \left| (\mathbf{D}^{\mathbf{k}} p_{t_*})(\mathbf{y}^{(i)}) \right| \left\{ 1 + D \delta^{-D_6 \log(1/\delta)} \{\log(1/\delta)\}^{(D-1)D_7 \log(1/\delta)} \right\} \tilde{\delta} \\ & \leq m^{\frac{\tau_{\text{sm}}(1-\tau_{\text{low}})+D}{D}} \delta^{-D_8 \log(1/\delta)} \tilde{\delta}, \quad h \in [D] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ . Let

$$\tilde{\delta} = \delta^{D_8 \log(1/\delta)} m^{-\frac{\tau_{\text{sm}}+D}{D}}$$

with large enough  $m$ . Combining (81) with the second last display, we have

$$\begin{aligned} |p_{t_*+t}(\mathbf{x}) - f_{t_*}(\mathbf{x}, t)| & \leq (1 + D_5) m^{-\frac{\tau_{\text{low}} \tau_{\text{sm}} - (D+1-\tau_{\text{low}}) D \bar{\tau} \tau_t}{D(1+D \bar{\tau} \tau_t)}} (\log m)^{D(\frac{\tau_{\text{sm}}}{2}+1)}, \\ \left| \sigma_t (\nabla p_{t_*+t}(\mathbf{x}))_h - \tilde{f}_{t_*}^{(h)}(\mathbf{x}, t) \right| & \leq (1 + D_5) m^{-\frac{\tau_{\text{low}} \tau_{\text{sm}} - (D+1-\tau_{\text{low}}) D \bar{\tau} \tau_t}{D(1+D \bar{\tau} \tau_t)}} (\log m)^{D(\frac{\tau_{\text{sm}}}{2}+1)}, \quad h \in [D] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \tau_x \sigma_t \sqrt{\log(1/\delta)}$  and  $\delta \leq t \leq \tau_t \log(1/\delta)$ . Consider a function  $\mathbf{f}_{t_*} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{D+1}$  such that  $\mathbf{f}_{t_*}(\mathbf{x}, t) = (f_{t_*}(\mathbf{x}, t), \tilde{f}_{t_*}^{(1)}(\mathbf{x}, t), \dots, \tilde{f}_{t_*}^{(D)}(\mathbf{x}, t))^\top$  for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . Lemma 9, Lemma 10, Lemma 11 and Lemma 12 implies that  $\mathbf{f}_{t_*} \in \mathcal{F}_{\text{NN}}(L, \mathbf{d}, s, m)$  with

$$\begin{aligned} L & \leq D_9 (\log m)^4, \quad \|\mathbf{d}\|_\infty \leq D_9 m (\log m)^9, \\ s & \leq D_9 m (\log m)^9, \quad M \leq \exp(D_9 (\log m)^2), \end{aligned}$$

where  $D_9 = D_9(D, \bar{\tau}, \underline{\tau}, \tau_t, \tau_x, \tau_{\text{sm}}, \tau_{\text{low}}, \tau_{\text{tail}}, C_{S,3}, C_{N,4}, C_{N,5}, D_7, D_8)$  is a large enough constant. The assertion follows by re-defining the constants.  $\blacksquare$

## B.5 Proof of Theorem 5

In this subsection, we provide the proof of Theorem 5 by combining Propositions 23 to 25.

*Proof of Theorem 5.* Let  $m > 0$  be a large enough value as described below and

$$D_1 = \sqrt{\frac{8\beta}{d}} \vee \sqrt{2\tau_{\min} + \frac{4\beta}{d}}.$$

We will approximate  $\nabla \log p_t(\mathbf{x})$  for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq \tau_{\max} \log m$  by neural networks by dividing the analysis into the following three cases:

1. (Interior of near-support)  $\|\mathbf{x}\|_\infty \leq \mu_t - \{\log(1/\sigma_t)\}^{-3/2}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$
2. (Boundary of near-support)  $\mu_t - \tau_{\min}^{3/2} \{(4D)^{3/2} + 3\} \{\log(1/\sigma_t)\}^{-3/2} \leq \|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$   
and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$
3. (large  $t$ )  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $2m^{-\frac{1}{2D}} \leq t \leq \tau_{\max} \log m$ .

Then, we combine the networks into a single network and derive the approximation error over the entire region  $(\mathbf{x}, t) \in \mathbb{R}^D \times [m^{-\tau_{\min}}, \tau_{\max} \log m]$ .

## B.5.1 INTERIOR OF NEAR-SUPPORT

Let  $\tau_{\text{tail}}^{(1)} = 4D\beta/d$  and  $\tau_{\text{bd}}^{(1)} = 3/2$ . Let

$$\begin{aligned}\tilde{C}_3 &= \tilde{C}_3(\beta, d, D, K, \bar{\tau}, \underline{\tau}, \tau_{\text{bd}}^{(1)}, \tau_{\text{tail}}^{(1)}, \tau_{\text{min}}), \\ \tilde{C}_4 &= \tilde{C}_4(\beta, d, D, K, \underline{\tau}, \tau_{\text{bd}}^{(1)}, \tau_{\text{tail}}^{(1)}, \tau_{\text{min}}), \\ \tilde{C}_5 &= \tilde{C}_5(\beta, d, \underline{\tau}, \tau_{\text{bd}}^{(1)}, \tau_{\text{tail}}^{(1)}, \tau_{\text{min}})\end{aligned}$$

be the constants in Proposition 23, where  $(\tau_{\text{tail}}, \tau_{\text{bd}})$  is replaced by  $(\tau_{\text{tail}}^{(1)}, \tau_{\text{bd}}^{(1)})$ . Also, let  $\tilde{C}_2 = \tilde{C}_2(\beta, D, \tau_{\text{bd}}^{(1)}, \tau_{\text{tail}}^{(1)})$  be the constant in Lemma 22, where  $(\tau_{\text{tail}}, \tau_{\text{bd}})$  is replaced by  $(\tau_{\text{tail}}^{(1)}, \tau_{\text{bd}}^{(1)})$ . For large enough  $m$  so that  $m \geq \tilde{C}_5$  and  $3m^{-1/(2D)} \leq \bar{\tau}^{-1}(\tilde{C}_2^2 \wedge 1/2)$ , Proposition 23 implies that there exists a collection of permutation matrices  $\mathcal{P}^{(1)} = (\mathcal{Q}_i^{(1)}, \mathcal{R}_i^{(1)})_{i \in [L-1]}$  and weight-sharing neural networks

$$\mathbf{f}^{(1)} = (f_1^{(1)}, \dots, f_{D+1}^{(1)})^\top \in \mathcal{F}_{\text{NN}}(L^{(1)}, \mathbf{d}^{(1)}, s^{(1)}, M^{(1)}, \mathcal{P}_{\mathbf{m}}^{(1)})$$

with

$$\begin{aligned}L^{(1)} &\leq \tilde{C}_3(\log m)^2 \log \log m, & \|\mathbf{d}^{(1)}\|_\infty &\leq \tilde{C}_3 m^{D+1}, \\ s^{(1)} &\leq \tilde{C}_3 m(\log m)^5 \log \log m, & M^{(1)} &\leq \exp(\tilde{C}_3 \{\log m\}^2), \\ \|\mathbf{m}^{(1)}\|_\infty &\leq \tilde{C}_3 m^D\end{aligned}$$

satisfying

$$\left\| \begin{pmatrix} \sigma_t \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} - \mathbf{f}^{(1)}(\mathbf{x}, t) \right\|_\infty \leq \tilde{C}_4 \left( 3^{\frac{2D\beta}{d}} + 1 \right) m^{-\frac{\beta}{d}} (\log m)^{2D+2\beta} \stackrel{\text{def}}{=} \epsilon_1$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t - \{\log(1/\sigma_t)\}^{-3/2}$  and  $m^{-\tau_{\text{min}}} \leq t \leq 3m^{-\frac{1}{2D}}$  because  $\mu_t \leq 1$ . Note that  $C_{S,1}^{-1} \leq p_t(\mathbf{x}) \leq C_{S,1}$  for  $\|\mathbf{x}\|_\infty \leq \mu_t$ ,  $t \geq 0$ , and  $\|\sigma_t \nabla p_t(\mathbf{x})\|_\infty \leq C_{S,3}$  for  $\mathbf{x} \in \mathbb{R}^D$ ,  $t \geq 0$ , where  $C_{S,1} = C_{S,1}(D, K, \tau_1)$  and  $C_{S,3} = C_{S,3}(D, K, \bar{\tau}, \underline{\tau})$  are the constants in Lemma 6 and Lemma 8, respectively. Also,  $C_{S,1}^{-1}/2 \leq p_t(\mathbf{x}) - \epsilon_1 \leq f_{D+1}^{(1)}(\mathbf{x}, t) \leq p_t(\mathbf{x}) + \epsilon_1 \leq 2C_{S,1}$  for  $\|\mathbf{x}\|_\infty \leq \mu_t - \mu_t \{\log(1/\sigma_t)\}^{-3/2}$  and  $m^{-\tau_{\text{min}}} \leq t \leq 3m^{-\frac{1}{2D}}$  with large enough  $m$  so that  $\epsilon_1 \leq C_{S,1}^{-1}/2$ . Let  $f_{\text{rec}}^{(\text{in})} \in \mathcal{F}_{\text{NN}}(L_{\text{rec}}^{(\text{in})}, \mathbf{d}_{\text{rec}}^{(\text{in})}, s_{\text{rec}}^{(\text{in})}, M_{\text{rec}}^{(\text{in})})$  be the neural networks in Lemma 19 with

$$\begin{aligned}L_{\text{rec}}^{(\text{in})} &\leq C_{N,5} \{\beta \log m/d\}^2, & \|\mathbf{d}_{\text{rec}}^{(\text{in})}\|_\infty &\leq C_{N,5} \{\beta \log m/d\}^3, \\ s_{\text{rec}}^{(\text{in})} &\leq C_{N,5} \{\beta \log m/d\}^4, & M_{\text{rec}}^{(\text{in})} &\leq C_{N,5} m^{\frac{2\beta}{d}}\end{aligned}$$

such that  $|1/x - f_{\text{rec}}^{(\text{in})}(x)| \leq m^{-\beta/d}$  for  $x \in [m^{-\beta/d}, m^{\beta/d}]$ . For large enough  $m$  so that  $m^{-\beta/d} \leq C_{S,1}^{-1}/2$ ,

$$\begin{aligned}&\left| \frac{1}{p_t(\mathbf{x})} - f_{\text{rec}}^{(\text{in})} \left( f_{D+1}^{(1)}(\mathbf{x}, t) \right) \right| \leq \left| \frac{1}{p_t(\mathbf{x})} - \frac{1}{f_{D+1}^{(1)}(\mathbf{x}, t)} \right| + \left| \frac{1}{f_{D+1}^{(1)}(\mathbf{x}, t)} - f_{\text{rec}}^{(\text{in})} \left( f_{D+1}^{(1)}(\mathbf{x}, t) \right) \right| \\ &\leq \{p_t(\mathbf{x}) \wedge f_{D+1}^{(1)}(\mathbf{x}, t)\}^{-2} \epsilon_1 + m^{-\frac{\beta}{d}} \leq (4C_{S,1}^2 + 1) \epsilon_1\end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t - \{\log(1/\sigma_t)\}^{-3/2}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ . Let

$$f_{\text{mult}}^{(\text{in})} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}^{(\text{in})}, \mathbf{d}_{\text{mult}}^{(\text{in})}, s_{\text{mult}}^{(\text{in})}, M_{\text{mult}}^{(\text{in})})$$

be the neural networks in Lemma 14 with

$$\begin{aligned} L_{\text{mult}}^{(\text{in})} &\leq C_{N,1} \log 2\{\beta \log m/d + 2 \log(C_{S,1} \vee C_{S,3}) + 2 \log 2\}, & \mathbf{d}_{\text{mult}}^{(\text{in})} &= (2, 96, \dots, 96, 1)^\top, \\ s_{\text{mult}}^{(\text{in})} &\leq C_{N,1} 2\{\beta \log m/d + \log(C_{S,1} \vee C_{S,3}) + \log 2\}, & M_{\text{mult}}^{(\text{in})} &= (C_{S,1} \vee C_{S,3})^2 \end{aligned}$$

such that  $|f_{\text{mult}}^{(\text{in})}(\tilde{\mathbf{x}}) - x_1 x_2| \leq m^{-\beta/d} + 2(C_{S,1} \vee C_{S,3})\tilde{\epsilon}$  for all  $\|\mathbf{x}\|_\infty \leq 2(C_{S,1} \vee C_{S,3})$ ,  $\tilde{\mathbf{x}} \in \mathbb{R}^2$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$  and  $|f_{\text{mult}}^{(\text{in})}(\mathbf{x})| \leq (C_{S,1} \vee C_{S,3})^2$  for all  $\mathbf{x} \in \mathbb{R}^2$ , where  $C_{N,1}$  is the constant in Lemma 14. Then,

$$\begin{aligned} &\left| \frac{\sigma_t (\nabla p_t(\mathbf{x}))_i}{p_t(\mathbf{x})} - f_{\text{mult}}^{(\text{in})} \left( f_i^{(1)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{in})} \left( f_{D+1}^{(1)}(\mathbf{x}, t) \right) \right) \right| \\ &\leq m^{-\frac{\beta}{d}} + 2(C_{S,1} \vee C_{S,3})(4C_{S,1}^2 + 1)\epsilon_1 \leq D_2 m^{-\frac{\beta}{d}} (\log m)^{2D+2\beta}, \quad i \in [D] \end{aligned} \quad (88)$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t - \{\log(1/\sigma_t)\}^{-3/2}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ , where  $D_2 = D_2(\beta, D, C_{S,1}, C_{S,3}, \tilde{C}_4)$ . Let  $0 < \delta \leq \underline{T} = m^{-\tau_{\min}}$  be a small enough value as described below. With  $\delta < 1/2$ , Lemma 18 implies that there exist neural networks  $f_\sigma \in \mathcal{F}_{\text{NN}}(L_\sigma, \mathbf{d}_\sigma, s_\sigma, M_\sigma)$  with

$$\begin{aligned} L_\sigma &\leq C_{N,4} \{\log(1/\delta)\}^2, & \|\mathbf{d}_\sigma\|_\infty &\leq C_{N,4} \{\log(1/\delta)\}^2 \\ s_\sigma &\leq C_{N,4} \{\log(1/\delta)\}^3, & M_\sigma &\leq C_{N,4} \log(1/\delta) \end{aligned} \quad (89)$$

such that  $|\sigma_t - f_\sigma(t)| \leq \delta$  for  $t \geq \delta$ , where  $C_{N,4}$  is the constant in Lemma 18. Also, Lemma 19 implies that there exists a neural network  $f_{\text{rec}} \in \mathcal{F}_{\text{NN}}(L_{\text{rec}}, \mathbf{d}_{\text{rec}}, s_{\text{rec}}, M_{\text{rec}})$  with

$$\begin{aligned} L_{\text{rec}} &\leq C_{N,5} \{\log(1/\delta)\}^2, & \|\mathbf{d}_{\text{rec}}\|_\infty &\leq C_{N,5} \{\log(1/\delta)\}^3 \\ s_{\text{rec}} &\leq C_{N,5} \{\log(1/\delta)\}^4, & M_{\text{rec}} &\leq C_{N,5} \delta^{-2} \end{aligned}$$

such that  $|1/x - f_{\text{rec}}(x)| \leq \delta$  for any  $x \in [\delta, 1/\delta]$ . Since  $\sigma_t - \delta \leq f_\sigma(t) \leq \sigma_t + \delta$  for  $t \geq \delta$  and  $\sqrt{\tau \underline{T}} \leq \sigma_t \leq 1$  for  $t \geq \underline{T}$ , we have  $\underline{T} \leq f_\sigma(t) \leq 2$  for  $t \geq \underline{T}$  with large enough  $m$  so that  $\underline{T} \leq \sqrt{\tau \underline{T}} - \underline{T}$  and  $\underline{T} \leq 1$ . Then,

$$\begin{aligned} |1/\sigma_t - f_{\text{rec}}(f_\sigma(t))| &\leq |1/\sigma_t - 1/f_\sigma(t)| + |1/f_\sigma(t) - f_{\text{rec}}(f_\sigma(t))| \\ &\leq \{\sigma_t \wedge f_\sigma(t)\}^{-2} |\sigma_t - f_\sigma(t)| + \delta \leq (1 + \underline{T}^{-2})\delta = (1 + m^{2\tau_{\min}})\delta \end{aligned} \quad (90)$$

for  $t \geq \underline{T}$ . Lemma 14 implies that there exists a neural network

$$f_{\text{mult}} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}, \mathbf{d}_{\text{mult}}, s_{\text{mult}}, M_{\text{mult}})$$

with

$$\begin{aligned} L_{\text{mult}} &\leq C_{N,1} \log 2\{\log(1/\delta) + 3DD_1^2 \log m\}, & \mathbf{d}_{\text{mult}} &= (2, 96, \dots, 96, 1)^\top, \\ s_{\text{mult}} &\leq C_{N,1} 2\{\log(1/\delta) + 3DD_1^2 \log m\}, & M_{\text{mult}} &= m^{6DD_1^2} \end{aligned}$$

such that

$$|f_{\text{mult}}(\tilde{x}_1, \tilde{x}_2) - x_1 x_2| \leq \delta + 2m^{3DD_1^2} \tilde{\epsilon} \quad (91)$$

for any  $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$  with  $\|\mathbf{x}\|_\infty \leq m^{3DD_1^2}$  and  $\tilde{\mathbf{x}} = (\tilde{x}_1, \tilde{x}_2) \in \mathbb{R}^k$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$ , where  $0 < \tilde{\epsilon} \leq 1$ . Consider functions  $\tilde{f}_1^{(1)}, \dots, \tilde{f}_D^{(1)} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\tilde{f}_i^{(1)}(\mathbf{x}, t) = f_{\text{mult}} \left( f_{\text{mult}}^{(\text{in})} \left( f_i^{(1)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{in})} \left( f_{D+1}^{(1)}(\mathbf{x}, t) \right) \right), f_{\text{rec}}(f_\sigma(t)) \right), \quad i \in [D]$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . For large enough  $m$  so that  $m^{3DD_1^2} \geq 4(C_{S,1} \vee C_{S,3})^2$ , we have

$$\begin{aligned} & \left| \sigma_t^{-1} f_{\text{mult}}^{(\text{in})} \left( f_i^{(1)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{in})} \left( f_{D+1}^{(1)}(\mathbf{x}, t) \right) \right) - \tilde{f}_i^{(1)}(\mathbf{x}, t) \right| \\ & \leq \delta + 2m^{3DD_1^2} (1 + m^{2\tau_{\min}}) \delta \leq 5m^{5DD_1^2} \delta, \quad i \in [D] \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq \underline{T}$  because  $D_1^2 \geq \tau_{\min}$ . Combining (88) with the last display, we have

$$\begin{aligned} & \left| (\nabla \log p_t(\mathbf{x}))_i - \tilde{f}_i^{(1)}(\mathbf{x}, t) \right| \sigma_t \\ & \leq \left| \frac{\sigma_t (\nabla p_t(\mathbf{x}))_i}{p_t(\mathbf{x})} - f_{\text{mult}}^{(\text{in})} \left( f_i^{(1)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{in})} \left( f_{D+1}^{(1)}(\mathbf{x}, t) \right) \right) \right| + 4m^{5DD_1^2} \delta \sigma_t \quad (92) \\ & \leq D_2 m^{-\frac{\beta}{d}} (\log m)^{2D+2\beta} + 4m^{5DD_1^2} \delta, \quad i \in [D] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t - \{\log(1/\sigma_t)\}^{-3/2}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ .

### B.5.2 BOUNDARY OF NEAR-SUPPORT

Let  $\delta^{(2)} = m^{-(3DD_1^2+2\beta/d)}$  and

$$\begin{aligned} \tau_{\text{bd}}^{(2)} &= 3/2, \quad \tilde{\tau}_{\text{bd}}^{(2)} = 1, \\ \tau_{\mathbf{x}}^{(2)} &= \left\{ \left( 3DD_1^2 + \frac{2\beta}{d} \right)^{-\frac{1}{2}} \vee 1 \right\} \left[ D_1 \vee \tau_{\min}^{\frac{3}{2}} \left\{ (4D)^{\frac{3}{2}} + 3 \right\} \right], \\ \tau_t^{(2)} &= \left\{ 3D \left( 3DD_1^2 + \frac{2\beta}{d} \right) \right\}^{-1} \wedge \frac{1}{2}. \end{aligned}$$

Let  $\tilde{C}_6 = \tilde{C}_6(D, K, \bar{\tau}, \underline{T}, \tau_{\mathbf{x}}^{(2)})$ ,  $\tilde{C}_7 = \tilde{C}_7(D, K, \underline{T})$ ,  $\tilde{C}_8 = \tilde{C}_8(D, \bar{\tau}, \tau_{\text{bd}}^{(2)}, \tau_{\mathbf{x}}^{(2)}, \tau_t^{(2)}, \tilde{\tau}_{\text{bd}}^{(2)})$  be the constants in Proposition 24, where  $(\tau_{\text{bd}}, \tilde{\tau}_{\text{bd}}, \tau_{\mathbf{x}}, \tau_t)$  is replaced by  $(\tau_{\text{bd}}^{(2)}, \tilde{\tau}_{\text{bd}}^{(2)}, \tau_{\mathbf{x}}^{(2)}, \tau_t^{(2)})$ . For large enough  $m$ , we have

$$\delta^{(2)} \leq \tilde{C}_8, \quad 3m^{-\frac{1}{2D}} \leq \left\{ \delta^{(2)} \right\}^{\tau_t^{(2)}}, \quad \left\{ \log(1/\delta^{(2)}) \right\}^{-\tilde{\tau}_{\text{bd}}^{(2)}} \leq \tau_2, \quad 2C_{S,1} m^{DD_1^2} \leq \left\{ \delta^{(2)} \right\}^{-1}.$$

Also, a simple calculation yields that

$$\delta^{(2)} \leq m^{-\tau_{\min}}, \quad \tau_{\mathbf{x}}^{(2)} \geq \tau_{\min}^{\frac{3}{2}} \left\{ (4D)^{\frac{3}{2}} + 3 \right\}, \quad D_1 \sqrt{\log m} \leq \tau_{\mathbf{x}}^{(2)} \sqrt{\log(1/\delta^{(2)})}.$$

Then, Proposition 24 implies that there exists a neural network

$$\mathbf{f}^{(2)} = (f_1^{(2)}, \dots, f_{D+1}^{(2)})^\top \in \mathcal{F}_{\text{NN}}(L^{(2)}, \mathbf{d}^{(2)}, s^{(2)}, M^{(2)})$$

with

$$\begin{aligned} L &\leq \tilde{C}_6 \left\{ \log \left( 1/\delta^{(2)} \right) \right\}^4, \quad \|\mathbf{d}\|_\infty \leq \tilde{C}_6 \left\{ \log \left( 1/\delta^{(2)} \right) \right\}^{7+2D}, \\ s &\leq \tilde{C}_6 \left\{ \log \left( 1/\delta^{(2)} \right) \right\}^{11+2D}, \quad M \leq \exp \left( \tilde{C}_6 \left\{ \log \left( 1/\delta^{(2)} \right) \right\}^2 \right), \end{aligned}$$

such that

$$\left\| \begin{pmatrix} \sigma_t \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} - \mathbf{f}^{(2)}(\mathbf{x}, t) \right\|_\infty \leq \tilde{C}_7 \delta^{(2)} \left\{ \log \left( 1/\delta^{(2)} \right) \right\}^D \stackrel{\text{def}}{=} \epsilon_2$$

for  $\mu_t - \tau_{\min}^{3/2} \{(4D)^{3/2} + 3\} \{\log(1/\sigma_t)\}^{-3/2} \leq \|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ . Lemma 6 implies that  $C_{S,1}^{-1} m^{-DD_1^2} \leq p_t(\mathbf{x}) \leq C_{S,1}$  for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $t \geq 0$ . Note that  $C_{S,1}^{-1} m^{-DD_1^2}/2 \leq p_t(\mathbf{x}) - \epsilon_2 \leq f_{D+1}^{(2)}(\mathbf{x}, t) \leq p_t(\mathbf{x}) + \epsilon_2 \leq 2C_{S,1}$  for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$  with large enough  $m$  so that  $\epsilon_2 \leq C_{S,1}^{-1} m^{-DD_1^2}/2$ . Let

$$f_{\text{rec}}^{(\text{bd})} \in \mathcal{F}_{\text{NN}}(L_{\text{rec}}^{(\text{bd})}, \mathbf{d}_{\text{rec}}^{(\text{bd})}, s_{\text{rec}}^{(\text{bd})}, M_{\text{rec}}^{(\text{bd})})$$

be the neural networks in Lemma 19 with

$$\begin{aligned} L_{\text{rec}}^{(\text{bd})} &\leq C_{N,5} \{\log(1/\delta^{(2)})\}^2, \quad \|\mathbf{d}_{\text{rec}}^{(\text{bd})}\|_\infty \leq C_{N,5} \{\log(1/\delta^{(2)})\}^3, \\ s_{\text{rec}}^{(\text{bd})} &\leq C_{N,5} \{\log(1/\delta^{(2)})\}^4, \quad M_{\text{rec}}^{(\text{bd})} \leq C_{N,5} \{\delta^{(2)}\}^{-2} \end{aligned}$$

such that  $|1/x - f_{\text{rec}}^{(\text{bd})}(x)| \leq \delta^{(2)}$  for  $x \in [\delta^{(2)}, 1/\delta^{(2)}]$ . Then,

$$\begin{aligned} &\left| \frac{1}{p_t(\mathbf{x})} - f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(2)}(\mathbf{x}, t) \right) \right| \leq \left| \frac{1}{p_t(\mathbf{x})} - \frac{1}{f_{D+1}^{(2)}(\mathbf{x}, t)} \right| + \left| \frac{1}{f_{D+1}^{(2)}(\mathbf{x}, t)} - f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(2)}(\mathbf{x}, t) \right) \right| \\ &\leq \{p_t(\mathbf{x}) \wedge f_{D+1}^{(2)}(\mathbf{x}, t)\}^{-2} \epsilon_2 + \delta^{(2)} \leq 4C_{S,1}^2 m^{2DD_1^2} \epsilon_2 + \delta^{(2)} \\ &\leq (4C_{S,1}^2 + 1) \epsilon_2 m^{2DD_1^2} \end{aligned}$$

for  $\mu_t - \tau_{\min}^{3/2} \{(4D)^{3/2} + 3\} \{\log(1/\sigma_t)\}^{-3/2} \leq \|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ . Let

$$f_{\text{mult}}^{(\text{bd})} \in \mathcal{F}_{\text{NN}}(L_{\text{mult}}^{(\text{bd})}, \mathbf{d}_{\text{mult}}^{(\text{bd})}, s_{\text{mult}}^{(\text{bd})}, M_{\text{mult}}^{(\text{bd})})$$

be the neural networks in Lemma 14 with

$$\begin{aligned} L_{\text{mult}}^{(\text{bd})} &\leq C_{N,1} \log 2 \{ (2\beta/d + 1 + 2DD_1^2) \log m + 2 \log(C_{S,1} \vee C_{S,3}) + 2 \log 2 \}, \\ \mathbf{d}_{\text{mult}}^{(\text{bd})} &= (2, 96, \dots, 96, 1)^\top, \\ s_{\text{mult}}^{(\text{bd})} &\leq C_{N,1} 2 \{ (2\beta/d + 1 + DD_1^2) \log m + \log(C_{S,1} \vee C_{S,3}) + \log 2 \}, \\ M_{\text{mult}}^{(\text{bd})} &= (C_{S,1} \vee C_{S,3})^2 m^{2DD_1^2} \end{aligned}$$

such that  $|f_{\text{mult}}^{(\text{bd})}(\tilde{\mathbf{x}}) - x_1 x_2| \leq m^{-2\beta/d-1} + 2(C_{S,1} \vee C_{S,3})m^{DD_1^2}\tilde{\epsilon}$  for all  $\|\mathbf{x}\|_\infty \leq (C_{S,1} \vee C_{S,3})m^{DD_1^2}$ ,  $\tilde{\mathbf{x}} \in \mathbb{R}^2$  with  $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq \tilde{\epsilon}$  and  $|f_{\text{mult}}^{(\text{bd})}(\mathbf{x})| \leq (C_{S,1} \vee C_{S,3})^2 m^{2DD_1^2}$  for all  $\mathbf{x} \in \mathbb{R}^2$ . Then,

$$\begin{aligned} & \left| \frac{\sigma_t(\nabla p_t(\mathbf{x}))_i}{p_t(\mathbf{x})} - f_{\text{mult}}^{(\text{bd})} \left( f_i^{(2)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(2)}(\mathbf{x}, t) \right) \right) \right| \\ & \leq m^{-2\beta/d-1} + 2(C_{S,1} \vee C_{S,3})(4C_{S,1}^2 + 1)\epsilon_2 m^{3DD_1^2} \leq D_3 m^{-2\beta/d} (\log m)^D, \quad i \in [D] \end{aligned} \quad (93)$$

for  $\mu_t - \tau_{\min}^{3/2} \{(4D)^{3/2} + 3\} \{\log(1/\sigma_t)\}^{-3/2} \leq \|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ , where  $D_3 = D_3(\beta, d, D, \tilde{C}_7, C_{S,1}, C_{S,3}, D_1)$ . Consider functions  $\tilde{f}_1^{(2)}, \dots, \tilde{f}_D^{(2)} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\tilde{f}_i^{(2)}(\mathbf{x}, t) = f_{\text{mult}} \left( f_{\text{mult}}^{(\text{bd})} \left( f_i^{(2)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(2)}(\mathbf{x}, t) \right) \right), f_{\text{rec}}(f_\sigma(t)) \right), \quad i \in [D]$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . For large enough  $m$  so that  $m^{3DD_1^2} \geq (C_{S,1} \vee C_{S,3})^2 m^{2DD_1^2}$ , (90) and (91) implies that

$$\begin{aligned} & \left| \sigma_t^{-1} f_{\text{mult}}^{(\text{bd})} \left( f_i^{(2)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(2)}(\mathbf{x}, t) \right) \right) - \tilde{f}_i^{(2)}(\mathbf{x}, t) \right| \\ & \leq \delta + 2m^{3DD_1^2} (1 + m^{2\tau_{\min}}) \delta \leq 5m^{5DD_1^2} \delta, \quad i \in [D] \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq m^{-\tau_{\min}}$ . Combining (93) with the last display, we have

$$\begin{aligned} & \left| (\nabla \log p_t(\mathbf{x}))_i - \tilde{f}_i^{(2)}(\mathbf{x}, t) \right| \sigma_t \\ & \leq \left| \frac{\sigma_t(\nabla p_t(\mathbf{x}))_i}{p_t(\mathbf{x})} - f_{\text{mult}}^{(\text{bd})} \left( f_i^{(2)}(\mathbf{x}, t), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(2)}(\mathbf{x}, t) \right) \right) \right| + 5m^{5DD_1^2} \delta \sigma_t \\ & \leq D_3 m^{-2\beta/d} (\log m)^D + 5m^{5DD_1^2} \delta \leq D_3 m^{-\beta/d} + 5m^{5DD_1^2} \delta, \quad i \in [D] \end{aligned} \quad (94)$$

for  $\mu_t - \tau_{\min}^{3/2} \{(4D)^{3/2} + 3\} \{\log(1/\sigma_t)\}^{-3/2} \leq \|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ , where the last inequality holds for large enough  $m$  so that  $(\log m)^D \leq m^{\beta/d}$ .

### B.5.3 LARGE $t$

Let  $m^{(3)} = \sqrt{m}$ ,  $\tau_{\text{low}}^{(3)} = 1/2$ ,

$$\begin{aligned} \tau_{\text{sm}}^{(3)} &= \left\{ \left[ \left( \frac{2D}{\tau_{\text{low}}^{(3)}} \right) (1+D) \left( \frac{2\beta}{d} + \frac{1}{2D} + 3DD_1^2 \right) + D \left( \frac{D+1-\tau_{\text{low}}^{(3)}}{\tau_{\text{low}}^{(3)}} \right) \right] \right. \\ & \quad \left. \vee \left[ D(1+D) \left( \frac{\{\tau_{\max} \bar{\tau}\} \vee \{1/2D\}}{\tau_{\text{low}}^{(3)}} \right) - \frac{D+1-\tau_{\text{low}}^{(3)}}{\tau_{\text{low}}^{(3)}} \right] \right\} + 1 \\ \tau_{\mathbf{x}}^{(3)} &= D_1 \left\{ \frac{2D(1+D)}{\tau_{\text{low}}^{(3)} \tau_{\text{sm}}^{(3)} + D + 1 - \tau_{\text{low}}^{(3)}} \right\}^{\frac{1}{2}}. \end{aligned}$$

Also, let

$$t_* = \left\{ m^{(3)} \right\}^{-\frac{2-2\tau_{\text{low}}^{(3)}}{D}}, \quad \delta^{(3)} = \left\{ m^{(3)} \right\}^{-\frac{\tau_{\text{low}}^{(3)} \tau_{\text{sm}}^{(3)} + D + 1 - \tau_{\text{low}}^{(3)}}{D(1+D)}},$$

and  $\tilde{C}_9, \tilde{C}_{10}, \tilde{C}_{11}$  be the constants in Proposition 25 depending on  $(D, K, \bar{\tau}, \mathcal{L}, \tau_x^{(3)}, \tau_{\text{sm}}^{(3)}, \tau_{\text{low}}^{(3)})$ , where  $(\tau_x, \tau_{\text{sm}}, \tau_{\text{low}})$  is replaced by  $(\tau_x^{(3)}, \tau_{\text{sm}}^{(3)}, \tau_{\text{low}}^{(3)})$ . A simple calculation yields that

$$\begin{aligned} t_* &= m^{-\frac{1}{2D}}, \quad \left\{ m^{(3)} \right\}^{-\frac{\tau_{\text{low}}^{(3)} \tau_{\text{sm}}^{(3)} - (D+1 - \tau_{\text{low}}^{(3)})D}{D(1+D)}} \leq m^{-\frac{2\beta}{d} - \frac{1}{2D} - 3DD_1^2}, \\ \tau_x^{(3)} \sqrt{\log(1/\delta^{(3)})} &= D_1 \sqrt{\log m}, \quad \delta^{(3)} \leq m^{-\frac{1}{2D}}, \quad \tau_{\text{max}} \log m \leq \bar{\tau}^{-1} \log(1/\delta^{(3)}). \end{aligned}$$

Also, for large enough  $m$ , we have

$$m^{(3)} \geq \tilde{C}_{11} \quad \text{and} \quad \left\{ \log m^{(3)} \right\}^{\frac{D\tau_{\text{sm}}^{(3)}}{2} + D} \leq m^{\frac{1}{4D}}.$$

Then, Proposition 25 implies that there exists a neural network

$$\mathbf{f}^{(3)} = (f_1^{(3)}, \dots, f_{D+1}^{(3)})^\top \in \mathcal{F}_{\text{NN}}(L^{(3)}, \mathbf{d}^{(3)}, s^{(3)}, M^{(3)})$$

with

$$\begin{aligned} L^{(3)} &\leq \tilde{C}_9 (\log m/2)^4, \quad \|\mathbf{d}^{(3)}\|_\infty \leq \tilde{C}_9 \sqrt{m} (\log m/2)^9, \\ s^{(3)} &\leq \tilde{C}_9 \sqrt{m} (\log m/2)^9, \quad M^{(3)} \leq \exp(\tilde{C}_9 \{\log m/2\}^2), \end{aligned}$$

such that

$$\left\| \begin{pmatrix} \sigma_{t-t_*} \nabla p_t(\mathbf{x}) \\ p_t(\mathbf{x}) \end{pmatrix} - \mathbf{f}^{(3)}(\mathbf{x}, t-t_*) \right\|_\infty \leq \tilde{C}_{10} 2^{-D(\tau_{\text{sm}}^{(3)}/2+1)} m^{-\frac{2\beta}{d} - \frac{1}{4D} - 3DD_1^2} \stackrel{\text{def}}{=} \epsilon_3$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $2m^{-\frac{1}{2D}} \leq t \leq \tau_{\text{max}} \log m$ , where  $t_* = m^{-1/(2D)}$ . Note that  $C_{S,1}^{-1} m^{-DD_1^2}/2 \leq p_t(\mathbf{x}) - \epsilon_3 \leq f_{D+1}^{(3)}(\mathbf{x}, t) \leq p_t(\mathbf{x}) + \epsilon_3 \leq 2C_{S,1}$  for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $2m^{-\frac{1}{2D}} \leq t \leq \tau_{\text{max}} \log m$  with large enough  $m$  so that  $\epsilon_3 \leq C_{S,1}^{-1} m^{-DD_1^2}/2$ . Then,

$$\begin{aligned} &\left| \frac{1}{p_t(\mathbf{x})} - f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(3)}(\mathbf{x}, t-t_*) \right) \right| \\ &\leq \left| \frac{1}{p_t(\mathbf{x})} - \frac{1}{f_{D+1}^{(3)}(\mathbf{x}, t-t_*)} \right| + \left| \frac{1}{f_{D+1}^{(3)}(\mathbf{x}, t-t_*)} - f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(3)}(\mathbf{x}, t-t_*) \right) \right| \\ &\leq \{p_t(\mathbf{x}) \wedge f_{D+1}^{(3)}(\mathbf{x}, t-t_*)\}^{-2} \epsilon_3 + \delta^{(2)} \leq 4C_{S,1}^2 \epsilon_3 m^{2DD_1^2} + \delta^{(2)} \\ &\leq (4C_{S,1}^2 + \tilde{C}_{10} 2^{-D(\tau_{\text{sm}}^{(3)}/2+1)}) \epsilon_3 m^{2DD_1^2} \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $2m^{-\frac{1}{2D}} \leq t \leq \tau_{\text{max}} \log m$ . The last inequality holds because  $2DD_1^2 \geq 4D\tau_{\text{min}} \geq 4/3 \geq 1/(4D)$ . Then,

$$\begin{aligned} &\left| \frac{\sigma_{t-t_*} (\nabla p_t(\mathbf{x}))_i}{p_t(\mathbf{x})} - f_{\text{mult}}^{(\text{bd})} \left( f_i^{(3)}(\mathbf{x}, t-t_*), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(3)}(\mathbf{x}, t-t_*) \right) \right) \right| \\ &\leq m^{-2\beta/d-1} + 2(C_{S,1} \vee C_{S,3}) (4C_{S,1}^2 + \tilde{C}_{10} 2^{-D(\tau_{\text{sm}}^{(3)}/2+1)}) \epsilon_3 m^{3DD_1^2} \leq D_4 m^{-\beta/d-1/(4D)} \end{aligned} \tag{95}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $2m^{-\frac{1}{2D}} \leq t \leq \tau_{\max} \log m$ . where  $D_4 = D_4(D, \tau_{\text{sm}}^{(3)}, \tilde{C}_{10}, C_{S,1}, C_{S,3})$ . Consider functions  $\tilde{f}_1^{(3)}, \dots, \tilde{f}_D^{(3)} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\tilde{f}_i^{(3)}(\mathbf{x}, t) = f_{\text{mult}} \left( f_{\text{mult}}^{(\text{bd})} \left( f_i^{(3)}(\mathbf{x}, t - t_*), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(3)}(\mathbf{x}, t - t_*) \right) \right), f_{\text{rec}}(f_\sigma(t - t_*)) \right), \quad i \in [D]$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . Combining with (90) and (91), we have

$$\begin{aligned} & \left| \sigma_{t-t_*}^{-1} f_{\text{mult}}^{(\text{bd})} \left( f_i^{(3)}(\mathbf{x}, t - t_*), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(3)}(\mathbf{x}, t - t_*) \right) \right) - \tilde{f}_i^{(3)}(\mathbf{x}, t) \right| \\ & \leq \delta + 2m^{3DD_1^2} (1 + m^{2\tau_{\min}}) \delta \leq 5m^{5DD_1^2} \delta, \quad i \in [D] \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 2m^{-1/(2D)}$ . Note that  $|\sigma_t/\sigma_{t-t_*}| \leq |\sigma_{t-t_*}^{-1}| \leq (2\mathcal{I})^{-1/2} m^{1/(4D)}$  for  $t \geq 2m^{-1/(2D)}$ . Combining (95) with the last display, we have

$$\begin{aligned} & \left| (\nabla \log p_t(\mathbf{x}))_i - \tilde{f}_i^{(3)}(\mathbf{x}, t) \right| \sigma_{t-t_*} \\ & \leq \left| \frac{\sigma_{t-t_*} (\nabla p_t(\mathbf{x}))_i}{p_t(\mathbf{x})} - f_{\text{mult}}^{(\text{bd})} \left( f_i^{(3)}(\mathbf{x}, t - t_*), f_{\text{rec}}^{(\text{bd})} \left( f_{D+1}^{(3)}(\mathbf{x}, t - t_*) \right) \right) \right| + 5m^{5DD_1^2} \delta \sigma_{t-t_*} \\ & \leq D_4 m^{-\beta/d - 1/(4D)} + 5m^{5DD_1^2} \delta, \quad i \in [D] \end{aligned}$$

and

$$\begin{aligned} & \left| (\nabla \log p_t(\mathbf{x}))_i - \tilde{f}_i^{(3)}(\mathbf{x}, t) \right| \sigma_t \\ & \leq \left| (\nabla \log p_t(\mathbf{x}))_i - \tilde{f}_i^{(3)}(\mathbf{x}, t) \right| \sigma_{t-t_*} (2\mathcal{I})^{-1/2} m^{1/(4D)} \\ & \leq D_4 (2\mathcal{I})^{-1/2} \sqrt{\mathcal{I}} m^{-\beta/d} + 5(2\mathcal{I})^{-1/2} \sqrt{\mathcal{I}} m^{5DD_1^2 + 1/(4D)} \delta, \quad i \in [D] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $2m^{-\frac{1}{2D}} \leq t \leq \tau_{\max} \log m$ . Let  $\delta = m^{-5DD_1^2 - 1/(4D) - \beta/d}$ . Then, there exists a positive constant  $D_5 = D_5(\mathcal{I}, D_2, D_3, D_4)$  such that (92), (94) and the last display are bounded by

$$D_5 m^{-\frac{\beta}{d}} (\log m)^{2D+2\beta} \stackrel{\text{def}}{=} \epsilon_4 \quad (96)$$

#### B.5.4 COMBINING INTO A SINGLE FUNCTION

For large enough  $m$  so that  $3m^{-1/(2D)} \leq (2\bar{\tau})^{-1}$ , we have

$$\{\log(1/\sqrt{\mathcal{I}}) + \tau_{\min} \log m/2\}^{-3/2} \leq \{\log(1/\sigma_t)\}^{-3/2} \leq \left\{ \log(1/\sqrt{6\bar{\tau}}) + \log m/(4D) \right\}^{-3/2}$$

for  $m^{-\tau_{\min}} \leq t \leq 3m^{-1/(2D)}$  because  $\sqrt{\mathcal{I}t} \leq \sigma_t \leq \sqrt{2\bar{\tau}t}$  for  $0 \leq t \leq (2\bar{\tau})^{-1}$ . For large enough  $m$  so that  $\log(1/\sqrt{\mathcal{I}}) \leq \tau_{\min} \log m/2$ , it follows that

$$\tau_{\min}^{-3/2} (\log m)^{-3/2} \leq \{\log(1/\sigma_t)\}^{-3/2} \leq (4D)^{3/2} (\log m)^{-3/2}$$

for  $m^{-\tau_{\min}} \leq t \leq 3m^{-1/(2D)}$ . Then,

$$\mu_t - \tau_{\min}^{3/2} \{(4D)^{3/2} + 3\} \{\log(1/\sigma_t)\}^{-3/2} < \mu_t - \bar{x} < \mu_t - \underline{x} < \mu_t - \{\log(1/\sigma_t)\}^{-3/2} \quad (97)$$

for  $m^{-\tau_{\min}} \leq t \leq 3m^{-1/(2D)}$ , where

$$\bar{x} = \{(4D)^{3/2} + 2\}(\log m)^{-3/2} \quad \text{and} \quad \underline{x} = \{(4D)^{3/2} + 1\}(\log m)^{-3/2}.$$

Consider piecewise linear functions  $f_{\text{swit},x}^{(1)}, f_{\text{swit},x}^{(2)} : \mathbb{R} \rightarrow [0, 1]$  such that

$$\begin{aligned} f_{\text{swit},x}^{(1)}(x) &= (\log m)^{3/2} \rho \left( -f_{\text{clip}}^{(\underline{x}, \bar{x})}(x) + \bar{x} \right) = \frac{1}{\bar{x} - \underline{x}} \max(-(x \vee \underline{x}) \wedge \bar{x} + \bar{x}, 0), \\ f_{\text{swit},x}^{(2)}(x) &= (\log m)^{3/2} \rho \left( f_{\text{clip}}^{(\underline{x}, \bar{x})}(x) - \underline{x} \right) = \frac{1}{\bar{x} - \underline{x}} \max((x \vee \underline{x}) \wedge \bar{x} - \underline{x}, 0), \end{aligned}$$

for  $x \in \mathbb{R}$ , where  $f_{\text{clip}}^{(\underline{x}, \bar{x})} \in \mathcal{F}_{\text{NN}}(2, (1, 2, 1)^\top, 7, \bar{x} \vee (\log m)^{3/2})$  is the neural network in Lemma 15. Note that  $f_{\text{swit},x}^{(1)}(x) + f_{\text{swit},x}^{(2)}(x) = 1$  for  $x \in \mathbb{R}$ , and  $f_{\text{swit},x}^{(1)}(x) = 0$  for  $x \geq \bar{x}$  and  $f_{\text{swit},x}^{(2)}(x) = 0$  for  $x \leq \underline{x}$ . Combining with (96) and (97), we have

$$\begin{aligned} & \left| f_{\text{swit},x}^{(1)}(\mu_t - f_{\max}(\mathbf{x})) \tilde{f}_i^{(1)}(\mathbf{x}, t) + f_{\text{swit},x}^{(2)}(\mu_t - f_{\max}(\mathbf{x})) \tilde{f}_i^{(2)}(\mathbf{x}, t) - (\nabla \log p_t(\mathbf{x}))_i \right| \\ & \leq \epsilon_4 / \sigma_t, \quad i \in [D] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ , where  $f_{\max} : \mathbb{R}^D \rightarrow \mathbb{R}$  is a function such that

$$\begin{aligned} f_{\max}(\mathbf{x}) &= \|\mathbf{x}\|_\infty \\ &= \rho(\cdots \rho(\rho(|x_1| - |x_2|) + |x_2| - |x_3|) + |x_3| - |x_4|) \cdots + |x_{D-1}| - |x_D|) + |x_D|. \end{aligned}$$

Note also that  $|x| = \rho(x) + \rho(-x)$ . Lemma 18 implies that there exist neural networks  $f_\mu \in \mathcal{F}_{\text{NN}}(L_\mu, \mathbf{d}_\mu, s_\mu, M_\mu)$  with

$$\begin{aligned} L_\mu &\leq C_{N,4} \{\log(1/\delta)\}^2, \quad \|\mathbf{d}_\mu\|_\infty \leq C_{N,4} \{\log(1/\delta)\}^2 \\ s_\mu &\leq C_{N,4} \{\log(1/\delta)\}^3, \quad M_\mu \leq C_{N,4} \log(1/\delta) \end{aligned}$$

such that  $|\mu_t - f_\mu(t)| \leq \delta$  for  $t \geq 0$ . Since  $f_{\text{swit},x}^{(1)}$  and  $f_{\text{swit},x}^{(2)}$  are  $(\log m)^{\tau_{\text{bd}}}$ -Lipschitz continuous,  $|f_{\text{swit},x}^{(i)}(\mu_t - \|\mathbf{x}\|_\infty) - f_{\text{swit},x}^{(i)}(f_\mu(t) - \|\mathbf{x}\|_\infty)| \leq \delta(\log m)^{\tau_{\text{bd}}}$  for each  $i \in \{1, 2\}$ ,  $\mathbf{x} \in \mathbb{R}^D$  and  $t \geq 0$ . For  $i \in [D]$ , consider a function  $f_i^{(x)} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$\begin{aligned} & f_i^{(x)}(\mathbf{x}, t) \\ &= f_{\text{mult}} \left( f_{\text{swit},x}^{(1)}(f_\mu(t) - f_{\max}(\mathbf{x})), \tilde{f}_i^{(1)}(\mathbf{x}, t) \right) + f_{\text{mult}} \left( f_{\text{swit},x}^{(2)}(f_\mu(t) - f_{\max}(\mathbf{x})), \tilde{f}_i^{(2)}(\mathbf{x}, t) \right) \end{aligned}$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . Combining with (91), we have

$$\begin{aligned} & \left| f_i^{(x)}(\mathbf{x}, t) - (\nabla \log p_t(\mathbf{x}))_i \right| \\ & \leq \epsilon_4 / \sigma_t + 2\delta + 4m^{3DD_1^2} \delta (\log m)^{\tau_{\text{bd}}} \leq \epsilon_4 / \sigma_t + 6m^{3DD_1^2} \delta (\log m)^{\tau_{\text{bd}}}, \quad i \in [D] \end{aligned} \tag{98}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq 3m^{-\frac{1}{2D}}$ . Similarly, let  $\underline{t} = 2m^{-\frac{1}{2D}}$  and  $\bar{t} = 3m^{-\frac{1}{2D}}$ , consider piecewise linear functions  $f_{\text{swit},t}^{(1)}, f_{\text{swit},t}^{(2)} : \mathbb{R} \rightarrow [0, 1]$  such that

$$\begin{aligned} f_{\text{swit},t}^{(1)}(t) &= m^{\frac{1}{2D}} \rho \left( -f_{\text{clip}}^{(\underline{t}, \bar{t})}(t) + \bar{t} \right) = \frac{1}{\bar{t} - \underline{t}} \max \left( -(t \vee \underline{t}) \wedge \bar{t} + \bar{t}, 0 \right), \\ f_{\text{swit},t}^{(2)}(t) &= m^{\frac{1}{2D}} \rho \left( f_{\text{clip}}^{(\underline{t}, \bar{t})}(t) - \underline{t} \right) = \frac{1}{\bar{t} - \underline{t}} \max \left( (t \vee \underline{t}) \wedge \bar{t} - \underline{t}, 0 \right), \end{aligned}$$

where  $f_{\text{clip}}^{(\underline{t}, \bar{t})} \in \mathcal{F}_{\text{NN}}(2, (1, 2, 1)^\top, 7, \bar{t} \vee m^{\frac{1}{2D}})$  is the neural network in Lemma 15. Note that  $f_{\text{swit},t}^{(1)}(t) + f_{\text{swit},t}^{(2)}(t) = 1$  for  $t \in \mathbb{R}$ , and  $f_{\text{swit},t}^{(1)}(t) = 0$  for  $t \geq \bar{t}$  and  $f_{\text{swit},t}^{(2)}(t) = 0$  for  $t \leq \underline{t}$ . Combining with (96) and (98), we have

$$\begin{aligned} & \left| f_{\text{swit},t}^{(1)}(t) f_i^{(\mathbf{x})}(\mathbf{x}, t) + f_{\text{swit},t}^{(2)}(t) \tilde{f}_i^{(3)}(\mathbf{x}, t) - (\nabla \log p_t(\mathbf{x}))_i \right| \\ & \leq \epsilon_4 / \sigma_t + 6m^{3DD_1^2} \delta(\log m)^{\tau_{\text{bd}}}, \quad i \in [D] \end{aligned}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq \tau_{\max} \log m$ . Consider a vector-valued function  $\mathbf{f}^{(\mathbf{x}, t)} = (f_1^{(\mathbf{x}, t)}, \dots, f_D^{(\mathbf{x}, t)}) : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}$  such that

$$f_i^{(\mathbf{x}, t)}(\mathbf{x}, t) = f_{\text{mult}} \left( f_{\text{swit},t}^{(1)}(t), f_i^{(\mathbf{x})}(\mathbf{x}, t) \right) + f_{\text{mult}} \left( f_{\text{swit},t}^{(2)}(t), \tilde{f}_i^{(3)}(\mathbf{x}, t) \right), \quad i \in [D]$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . Combining with (91), we have

$$\begin{aligned} & \left| f_i^{(\mathbf{x}, t)}(\mathbf{x}, t) - (\nabla \log p_t(\mathbf{x}))_i \right| \leq \epsilon_4 / \sigma_t + 6m^{3DD_1^2} \delta(\log m)^{\tau_{\text{bd}}} + 4\delta \\ & \leq \epsilon_4 / \sigma_t + 10m^{3DD_1^2} \delta(\log m)^{\tau_{\text{bd}}} \leq 11\epsilon_4 / \sigma_t, \quad i \in [D] \end{aligned} \tag{99}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq \tau_{\max} \log m$ , where the last inequality holds with large enough  $m$  so that  $m^{3DD_1^2} \delta(\log m)^{\tau_{\text{bd}}} \leq \epsilon_4$ . Since  $\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_2$  for any  $\mathbf{x} \in \mathbb{R}^D$ , Lemma 7 implies that  $\sigma_t \|\nabla \log p_t(\mathbf{x})\|_\infty \leq C_{S,2} D_1 \sqrt{\log m}$  for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $t \geq 0$  with large enough  $m$  so that  $D_1 \sqrt{\log m} \geq 1$ , where  $C_{S,2} = C_{S,2}(D, K, \tau_1, \bar{\tau}, \underline{\tau})$  is the constant in Lemma 7. Combining with the last display, we have

$$\sigma_t \left| f_i^{(\mathbf{x}, t)}(\mathbf{x}, t) \right| \leq 11\epsilon_4 + C_{S,2} D_1 \sqrt{\log m} \leq D_6 \sqrt{\log m}, \quad i \in [D]$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq \tau_{\max} \log m$  with large enough  $m$  so that  $\epsilon_4 \leq \sqrt{\log m}$ , where  $D_6 = D_6(\beta, d, D, C_{S,2})$ . Consider a function  $\mathbf{f} = (f_1, \dots, f_D)^\top : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^D$  such that

$$f_i(\mathbf{x}, t) = \left( f_i^{(\mathbf{x}, t)}(\mathbf{x}, t) \vee -\sigma_t^{-1} D_6 \sqrt{\log m} \right) \wedge \sigma_t^{-1} D_6 \sqrt{\log m}, \quad i \in [D]$$

for  $\mathbf{x} \in \mathbb{R}^D$  and  $t \in \mathbb{R}$ . Note that  $f_i(\mathbf{x}, t) = f_i^{(\mathbf{x}, t)}(\mathbf{x}, t)$  for  $i \in [D]$ ,  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq \tau_{\max} \log m$ . Combining with (99),

$$\sigma_t \|\mathbf{f}(\mathbf{x}, t) - \nabla \log p_t(\mathbf{x})\|_\infty \leq 11\epsilon_4 = 11D_5 m^{-\frac{\beta}{d}} (\log m)^{2D+2\beta} \tag{100}$$

for  $\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}$  and  $m^{-\tau_{\min}} \leq t \leq \tau_{\max} \log m$ .

## B.5.5 OUTSIDE OF NEAR-SUPPORT

Note that

$$\begin{aligned}
 & \int_{\underline{T}}^{\bar{T}} \int_{\mathbb{R}^D} \|\nabla \log p_t(\mathbf{x}) - \mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \\
 & \leq \int_{\underline{T}}^{\bar{T}} \int_{\|\mathbf{x}\|_\infty \leq \mu_t + \sigma_t D_1 \sqrt{\log m}} \|\nabla \log p_t(\mathbf{x}) - \mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \\
 & \quad + \int_{\underline{T}}^{\bar{T}} \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \|\nabla \log p_t(\mathbf{x}) - \mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x}
 \end{aligned}$$

For  $t \geq 0$ ,

$$\begin{aligned}
 & \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} p_t(\mathbf{x}) d\mathbf{x} = \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} d\mathbf{x} \\
 & = \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \int_{\|\sigma_t \mathbf{z} + \mu_t \mathbf{y}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y} \\
 & \leq \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \sum_{i=1}^D \int_{|\sigma_t z_i + \mu_t y_i| \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y} \\
 & \leq \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \sum_{i=1}^D \int_{|z_i| \geq D_1 \sqrt{\log m}} \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y} = D \int_{|z| \geq D_1 \sqrt{\log m}} \phi(z) dz,
 \end{aligned}$$

where the last inequality holds because  $|y_i| \leq 1$ . By the tail probability of the standard normal distribution, the last display is bounded by

$$2Dm^{-D_1^2/2}. \quad (101)$$

Let  $C_{S,2} = C_{S,2}(D, K, \tau_1, \bar{\tau}, \underline{\tau})$  be the constant in Lemma 7. Then,  $\|\nabla \log p_t(\mathbf{x})\|_2 \leq C_{S,2}(\|\mathbf{x}\|_\infty - \mu_t)/\sigma_t^2$  for  $\|\mathbf{x}\|_\infty \geq \mu_t + D_1 \sqrt{\log m}$  with large enough  $m$  so that  $D_1 \sqrt{\log m} \geq 1$ . Combining with the last display, we have

$$\begin{aligned}
 & \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \|\nabla \log p_t(\mathbf{x})\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \\
 & \leq 2C_{S,2}^2 \sigma_t^{-4} \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} (\|\mathbf{x}\|_\infty^2 + \mu_t^2) p_t(\mathbf{x}) d\mathbf{x} \\
 & \leq 2C_{S,2}^2 \sigma_t^{-4} \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \|\mathbf{x}\|_2^2 p_t(\mathbf{x}) d\mathbf{x} + 2DC_{S,2}^2 \sigma_t^{-4} \mu_t^2 m^{-D_1^2/2}
 \end{aligned}$$

for  $t \geq 0$ . A simple calculation yields that

$$\begin{aligned}
 & \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \|\mathbf{x}\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \\
 &= \sum_{i=1}^D \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} x_i^2 \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{x} d\mathbf{y} \\
 &= \sum_{i=1}^D \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \int_{\|\sigma_t \mathbf{z} + \mu_t \mathbf{y}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} (\sigma_t z_i + \mu_t y_i)^2 \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y} \\
 &\leq \sum_{i=1}^D \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \int_{\|\sigma_t \mathbf{z} + \mu_t \mathbf{y}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} 2(\sigma_t^2 z_i^2 + \mu_t^2 y_i^2) \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y} \\
 &\leq \sum_{i=1}^D \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \sum_{j=1}^D \int_{|\sigma_t z_j + \mu_t y_j| \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} 2(\sigma_t^2 z_i^2 + \mu_t^2 y_i^2) \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y}
 \end{aligned}$$

for  $t \geq 0$ . Since  $|y_j| \leq 1$  in the last integral, the last display is bounded by

$$\begin{aligned}
 & \sum_{i=1}^D \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \sum_{j=1}^D \int_{|z_j| \geq D_1 \sqrt{\log m}} 2(\sigma_t^2 z_i^2 + \mu_t^2 y_i^2) \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y} \\
 &\leq 2\sigma_t^2 \sum_{i=1}^D \sum_{j=1}^D \int_{|z_j| \geq D_1 \sqrt{\log m}} z_i^2 \phi_1(\mathbf{z}) d\mathbf{z} + 4D^2 \mu_t^2 m^{-D_1^2/2},
 \end{aligned}$$

where the last inequality holds by (101). Furthermore,

$$\begin{aligned}
 & \sum_{i=1}^D \sum_{j=1}^D \int_{|z_j| \geq D_1 \sqrt{\log m}} z_i^2 \phi_1(\mathbf{z}) d\mathbf{z} \\
 &= \sum_{i=1}^D \left\{ (D-1) \mathbb{E}[Z^2] \int_{|z| \geq D_1 \sqrt{\log m}} \phi(z) dz + \int_{|z| \geq D_1 \sqrt{\log m}} z^2 \phi(z) dz \right\} \\
 &\leq 2D \left\{ (D-1) m^{-D_1^2/2} + \sqrt{\mathbb{E}[Z^4]} m^{-D_1^2/4} \right\} \leq 2D(D + \sqrt{3} - 1) m^{-D_1^2/4},
 \end{aligned}$$

where the first inequality holds by the Cauchy-Schwarz inequality. Hence, there exists a constant  $D_7 = D_7(D, \underline{\tau}, C_{S,2})$  such that

$$\int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \|\nabla \log p_t(\mathbf{x})\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \leq D_7 \sigma_t^{-2} m^{-2\beta/d}$$

for  $t \geq m^{-\tau_{\min}}$  because  $\mu_t \leq 1$  and  $\sigma_t \geq \sqrt{\underline{\tau} m^{-\tau_{\min}}}$ . Combining with (101), we have

$$\begin{aligned}
 & \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} \|\nabla \log p_t(\mathbf{x}) - \mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \\
 &\leq \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} 2\|\nabla \log p_t(\mathbf{x})\|_2^2 p_t(\mathbf{x}) d\mathbf{x} + \int_{\|\mathbf{x}\|_\infty \geq \mu_t + \sigma_t D_1 \sqrt{\log m}} 2\|\mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \\
 &\leq 2D_7 \sigma_t^{-2} m^{-2\beta/d} + 4\sigma_t^{-2} D^2 D_6^2 m^{-D_1^2/2} \log m \\
 &\leq \sigma_t^{-2} \left( 2D_7 m^{-2\beta/d} + 4D^2 D_6^2 m^{-2\beta/d} \log m \right)
 \end{aligned}$$

for  $t \geq m^{-\tau_{\min}}$ , where the second inequality holds because  $\|\mathbf{f}(\mathbf{x}, t)\|_{\infty} \leq \sigma_t^{-1} D_6 \sqrt{\log m}$  for  $\mathbf{x} \in \mathbb{R}^D, t \in \mathbb{R}$ . Combining with (100), we have

$$\begin{aligned} & \sigma_t^2 \int_{\mathbb{R}^D} \|\nabla \log p_t(\mathbf{x}) - \mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} \\ & \leq D_{11}^2 D_5^2 m^{-\frac{2\beta}{d}} (\log m)^{4D+4\beta} + 2D_7 m^{-\frac{2\beta}{d}} + 4D^2 D_6^2 m^{-D_1^2/2} \log m \\ & \leq D_8 m^{-\frac{2\beta}{d}} (\log m)^{4D+4\beta} \end{aligned}$$

for  $m^{-\tau_{\min}} \leq t \leq \tau_{\max} \log m$ , where  $D_8 = D_7(D, D_5, D_6, D_7)$ . Since  $\sigma_t^2 \geq \underline{\tau} t$  for  $t \geq 0$ , we have

$$\begin{aligned} & \int_{\underline{T}}^{\bar{T}} \int_{\mathbb{R}^D} \|\nabla \log p_t(\mathbf{x}) - \mathbf{f}(\mathbf{x}, t)\|_2^2 p_t(\mathbf{x}) d\mathbf{x} dt \\ & \leq D_8 \underline{\tau}^{-1} m^{-\frac{2\beta}{d}} (\log m)^{4D+4\beta} (\log \bar{T} - \log \underline{T}) \\ & \leq D_9 m^{-\frac{2\beta}{d}} (\log m)^{4D+4\beta+1}, \end{aligned}$$

where  $D_9 = D_9(\underline{\tau}, \tau_{\max}, \tau_{\min}, D_8)$ . Lemma 9, Lemma 10, Lemma 11, Lemma 12 and Lemma 13 imply that  $\mathbf{f}^{(\mathbf{x}, t)} \in \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, m, M, \mathcal{P})$  with

$$\begin{aligned} L & \leq D_{10} (\log m)^6 \log \log m, \quad \|\mathbf{d}\|_{\infty} \leq D_{10} m^{D+1}, \\ s & \leq D_{10} m (\log m)^5 \log \log m, \quad M \leq \exp(D_{10} \{\log m\}^6), \end{aligned}$$

$\|\mathbf{m}\|_{\infty} \leq D_{10} m^D$  and the set of permutation matrices  $\mathcal{P}$ , where

$$D_{10} = D_{10}(\beta, d, D, \tau_{\min}, \tilde{C}_3, \tilde{C}_6, \tilde{C}_9, C_{N,1}, C_{N,4}, C_{N,5}, C_{S,1}, D_1)$$

is a large enough constant. The assertion follows by re-defining the constants.  $\blacksquare$

## Appendix C. Proofs for the Convergence Rate

In this section, we provide the proof of Theorem 3. We begin by outlining auxiliary lemmas and a proposition.

**Lemma 26 (Error bound for small  $t$ )** *Let  $\beta, K > 0$  be given and suppose the true density  $p_0$  belongs to  $\mathcal{H}^{\beta, K}([-1, 1]^D)$ . Then, there exist positive constants  $\tilde{C}_{12} = \tilde{C}_{12}(\beta, D, K, \bar{\tau}, \underline{\tau})$  and  $\tilde{C}_{13} = \tilde{C}_{13}(\bar{\tau}, \underline{\tau})$  such that*

$$\int_{\mathbb{R}^D} |p_0(\mathbf{x}) - p_t(\mathbf{x})| d\mathbf{x} \leq \tilde{C}_{12} \{t \log(1/t)\}^{\frac{\beta \wedge 1}{2}}$$

for  $0 < t \leq \tilde{C}_{13}$ .

For any function  $\mathbf{f} : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{n_2}, n_1, n_2 \in \mathbb{N}$  and  $C > 0$ , denote  $\|\cdot\|_{L^{\infty}([-C, C]^{n_1})}$  as the sup-norm over  $[-C, C]^{n_1}$ , defined as

$$\|\mathbf{f}\|_{L^{\infty}([-C, C]^{n_1})} = \sup_{\mathbf{x} \in [-C, C]^{n_1}} \|\mathbf{f}(\mathbf{x})\|_{\infty}.$$

For a function space  $\mathcal{F}$ ,  $N(\delta, \mathcal{F}, d)$  denotes the covering numbers with respect to the (pseudo)-metric  $d$ ; see van der Vaart and Wellner (1996) for the detailed definition. The following lemma provides a covering number of  $\mathcal{F}_{\text{WSNN}}$ . Our main proof strategy follows the proof of Lemma 5 from Schmidt-Hieber (2020), with modifications for weight-sharing networks.

**Lemma 27 (Covering number of  $\mathcal{F}_{\text{WSNN}}$ )** *Let  $C$  and  $0 < \delta < 1$  be given. For the class of weight-sharing neural networks  $\mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$ , we have*

$$\begin{aligned} & \log N\left(\delta, \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}}), \|\cdot\|_{L^\infty([-C, C]^{d_1})}\right) \\ & \leq (s+1) \log\left(\frac{4L^2 \|\mathbf{d}\|_\infty^2 \{\|\mathbf{m}\|_\infty \|\mathbf{d}\|_\infty (M \vee 1)\}^L (L+C+3)}{\delta}\right). \end{aligned}$$

For  $\underline{T}, \bar{T} > 0$  with  $\underline{T} < \bar{T}$  and a function  $\mathbf{f} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^D$ , recall the definition of loss function  $\ell_{\mathbf{f}} : [-1, 1]^D \rightarrow \mathbb{R}$ , given by

$$\begin{aligned} \ell_{\mathbf{f}}(\mathbf{x}) &= \int_{\underline{T}}^{\bar{T}} \mathbb{E}\left[\left\|\mathbf{f}(\mathbf{X}_t, t) + \frac{\mathbf{X}_t - \mu_t \mathbf{X}_0}{\sigma_t^2}\right\|_2^2 \mid \mathbf{X}_0 = \mathbf{x}\right] dt \\ &= \int_{\underline{T}}^{\bar{T}} \mathbb{E}\left[\left\|\mathbf{f}(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{\mathbf{Z}}{\sigma_t}\right\|_2^2\right] dt, \end{aligned}$$

where the last equality holds because  $\mathbf{X}_t = \mu_t \mathbf{X}_0 + \sigma_t \mathbf{Z}$  with  $D$ -dimensional standard normal variable  $\mathbf{Z}$ . Define the pointwise excess risk by

$$\nu_{\mathbf{f}}(\mathbf{x}) = \ell_{\mathbf{f}}(\mathbf{x}) - \ell_{\mathbf{f}_0}(\mathbf{x}),$$

where  $(\mathbf{x}, t) \mapsto \mathbf{f}_0(\mathbf{x}, t) = \nabla \log p_t(\mathbf{x})$  is a score function. Combining with (5), we have

$$\mathbb{E}[\nu_{\mathbf{f}}(\mathbf{X}_0)] = \int_{\underline{T}}^{\bar{T}} \mathbb{E}\left[\left\|\mathbf{f}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t)\right\|_2^2\right] dt.$$

The following lemma provides an upper bound on the sup-norm and the second moment (hence a variance-type bound) of the excess risk over the bounded function class.

**Lemma 28 (Upper bounds of excess risk)** *Let  $K, \tau_1, F, \underline{T}, \bar{T} > 0$  be given and suppose the true density  $p_0$  satisfies that  $\tau_1 \leq p_0(\mathbf{x}) \leq K$  for any  $\mathbf{x} \in [-1, 1]^D$ . For any function  $\mathbf{f} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^D$  satisfying  $\|\mathbf{f}(\cdot, t)\|_{L^\infty(\mathbb{R}^D)} \leq F\sigma_t^{-1}$  for all  $t \in [\underline{T}, \bar{T}]$ , there exists a positive constant  $\tilde{C}_{14} = \tilde{C}_{14}(D, K, \tau_1, \bar{\tau}, \underline{\tau})$  such that*

$$\|\nu_{\mathbf{f}}\|_{L^\infty([-1, 1]^D)} \leq \tilde{C}_{14}(F^2 \vee 1) (\log \bar{T} - \log \underline{T})$$

and

$$\mathbb{E}\left[\{\nu_{\mathbf{f}}(\mathbf{X}_0)\}^2\right] \leq 2\tilde{C}_{14}(F^2 \vee 1) (\log \bar{T} - \log \underline{T}) \mathbb{E}[\nu_{\mathbf{f}}(\mathbf{X}_0)].$$

The following proposition provides an oracle inequality for the ERM estimator under the score-matching loss. The statement is similar to Theorem C.4 from Oko et al. (2023) while addressing the issue identified by Yakovlev and Puchkin (2025). Our main proof strategy follows the proof of Proposition 12 from Stéphanovitch et al. (2025) with modifications that control the excess risk variance.

**Proposition 29 (Oracle inequality for score matching)** *Let  $K, \tau_1, F, \underline{T}, \bar{T} > 0$  be given and suppose the true density  $p_0$  satisfies that  $\tau_1 \leq p_0(\mathbf{x}) \leq K$  for any  $\mathbf{x} \in [-1, 1]^D$ . Let  $\mathbf{X}^1, \dots, \mathbf{X}^n$  be the i.i.d. samples drawn from  $p_0$ . For the class  $\mathcal{F}$ , consisting of continuous functions  $\mathbf{f} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^D$  with  $\|\mathbf{f}(\cdot, t)\|_{L^\infty(\mathbb{R}^D)} \leq F\sigma_t^{-1}$  for all  $t \in [\underline{T}, \bar{T}]$ , let*

$$\hat{\mathbf{f}} \in \operatorname{argmin}_{\mathbf{f} \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \ell_{\mathbf{f}}(\mathbf{X}^i)$$

be the ERM estimator over the class  $\mathcal{F}$ . Then, there exists a positive constant  $\tilde{C}_{14} = \tilde{C}_{14}(D, K, \tau_1, \bar{\tau}, \underline{\tau})$  such that

$$\begin{aligned} & \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \left\| \hat{\mathbf{f}}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t) \right\|_2^2 \right] dt \\ & \leq 3 \inf_{\mathbf{f} \in \mathcal{F}} \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \left\| \mathbf{f}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t) \right\|_2^2 \right] dt \\ & \quad + \frac{\bar{C}_1}{n} \left\{ \log N \left( n^{-2}, \mathcal{F}, \|\cdot\|_{L^\infty([- \bar{C}_2, \bar{C}_2]^{D+1})} \right) + \log(2n) \right\}, \end{aligned}$$

where

$$\bar{C}_1 = \tilde{C}_{14}(F^2 \vee 1) \left( \sqrt{\bar{T}} + \sqrt{\log \bar{T} - \log \underline{T}} \right) \left( \sqrt{\log \bar{T} - \log \underline{T}} \right)$$

and

$$\bar{C}_2 = \left( 1 + 2\sqrt{2 \log n} \right) \vee \bar{T}.$$

### C.1 Proof of Lemma 26

**Proof** Note that  $p_0$  is continuous and supported on  $[-1, 1]^D$ . Thus, for  $t \geq 0$ ,

$$\int_{\mathbb{R}^D} |p_0(\mathbf{x}) - p_t(\mathbf{x})| d\mathbf{x} = \int_{\|\mathbf{x}\|_\infty \leq 1} |p_0(\mathbf{x}) - p_t(\mathbf{x})| d\mathbf{x} + \int_{\|\mathbf{x}\|_\infty \geq 1} p_t(\mathbf{x}) d\mathbf{x}.$$

We will derive error bounds for each integral on the RHS.

Note that  $p_0 \in \mathcal{H}^{\beta, K}([-1, 1]^D)$ . If  $\beta \leq 1$ ,  $|p_0(\mathbf{x}) - p_0(\mathbf{y})| \leq K\|\mathbf{x} - \mathbf{y}\|_\infty^\beta$  for any  $\mathbf{x}, \mathbf{y} \in [-1, 1]^D$  by the definition of  $\mathcal{H}^{\beta, K}$ . If  $\beta > 1$ , Mean value theorem implies that  $|p_0(\mathbf{x}) - p_0(\mathbf{y})| \leq K\|\mathbf{x} - \mathbf{y}\|_2$  for any  $\mathbf{x}, \mathbf{y} \in [-1, 1]^D$ . Combining two cases, we have

$$|p_0(\mathbf{x}) - p_0(\mathbf{y})| \leq K\sqrt{D}\|\mathbf{x} - \mathbf{y}\|_\infty^{\beta \wedge 1}, \quad \forall \mathbf{x}, \mathbf{y} \in [-1, 1]^D. \quad (102)$$

A simple calculation yields that for any  $\mathbf{x} \in [-1, 1]^D$ ,

$$\begin{aligned} & p_0(\mathbf{x}) - p_t(\mathbf{x}) \\ &= \int_{\|\mathbf{y}\|_\infty \leq 1} \{p_0(\mathbf{x}) - p_0(\mathbf{y})\} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} + p_0(\mathbf{x}) \left( 1 - \int_{\|\mathbf{y}\|_\infty \leq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right). \end{aligned}$$

Then, for any  $t \geq 0$ ,

$$\begin{aligned} & \int_{\|\mathbf{x}\|_\infty \leq 1} |p_0(\mathbf{x}) - p_t(\mathbf{x})| d\mathbf{x} \\ & \leq \int_{\|\mathbf{x}\|_\infty \leq 1} \left| \int_{\|\mathbf{y}\|_\infty \leq 1} \{p_0(\mathbf{x}) - p_0(\mathbf{y})\} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| d\mathbf{x} \\ & \quad + \int_{\|\mathbf{x}\|_\infty \leq 1} p_0(\mathbf{x}) \left| 1 - \int_{\|\mathbf{y}\|_\infty \leq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| d\mathbf{x} \end{aligned} \quad (103)$$

We bound each term on the RHS. For any  $\delta > 0$ , a simple calculation yields that

$$\begin{aligned} & \int_{\|\mathbf{x}\|_\infty \leq 1} \left| \int_{\|\mathbf{y}\|_\infty \leq 1} \{p_0(\mathbf{x}) - p_0(\mathbf{y})\} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right| d\mathbf{x} \\ & \leq K\sqrt{D} \int_{\|\mathbf{x}\|_\infty \leq 1} \int_{\|\mathbf{y}\|_\infty \leq 1} \|\mathbf{x} - \mathbf{y}\|_\infty^{\beta\wedge 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} d\mathbf{x} \\ & \leq K\sqrt{D} \int_{\|\mathbf{x}\|_\infty \leq 1} \left( \delta^{\beta\wedge 1} \int_{\substack{\|\mathbf{y}\|_\infty \leq 1 \\ \|\mathbf{x} - \mathbf{y}\|_\infty \leq \delta}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} + 2^{\beta\wedge 1} \int_{\substack{\|\mathbf{y}\|_\infty \leq 1 \\ \|\mathbf{x} - \mathbf{y}\|_\infty \geq \delta}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} \right) d\mathbf{x} \\ & \leq K\sqrt{D} 2^D \mu_t^{-D} \delta^{\beta\wedge 1} + K\sqrt{D} 2^{\beta\wedge 1} \int_{\|\mathbf{x}\|_\infty \leq 1} \int_{\substack{\|\mathbf{y}\|_\infty \leq 1 \\ \|\mathbf{x} - \mathbf{y}\|_\infty \geq \delta}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} d\mathbf{x}, \end{aligned} \quad (104)$$

where the first inequality holds by (102) and the last inequality holds because

$$\int_{\mathbb{R}^D} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} = \mu_t^{-D}, \quad \forall \mathbf{x} \in \mathbb{R}^D. \quad (105)$$

Since  $1 - \mu_t \geq 0$ , we have  $\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \geq \|\mathbf{x} - \mathbf{y}\|_\infty - (1 - \mu_t)\|\mathbf{y}\|_\infty \geq \delta - (1 - \mu_t)$  for  $\|\mathbf{x} - \mathbf{y}\|_\infty \geq \delta$  and  $\|\mathbf{y}\|_\infty \leq 1$ . Then, a simple calculation yields that

$$\begin{aligned} & \int_{\|\mathbf{x}\|_\infty \leq 1} \int_{\substack{\|\mathbf{y}\|_\infty \leq 1 \\ \|\mathbf{x} - \mathbf{y}\|_\infty \geq \delta}} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} d\mathbf{x} \leq \int_{\|\mathbf{x}\|_\infty \leq 1} \int_{\|\mathbf{x} - \mu_t \mathbf{y}\|_\infty \geq \delta - (1 - \mu_t)} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} d\mathbf{x} \\ & = \mu_t^{-D} \int_{\|\mathbf{x}\|_\infty \leq 1} \int_{\|\mathbf{z}\|_\infty \geq \frac{\delta - (1 - \mu_t)}{\sigma_t}} \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{x} = 2^D \mu_t^{-D} \int_{\|\mathbf{z}\|_\infty \geq \frac{\delta - (1 - \mu_t)}{\sigma_t}} \phi_1(\mathbf{z}) d\mathbf{z} \\ & \leq 2^D \mu_t^{-D} \sum_{i=1}^D \int_{|z_i| \geq \frac{\delta - (1 - \mu_t)}{\sigma_t}} \phi_1(\mathbf{z}) d\mathbf{z} \leq D 2^{D+1} \mu_t^{-D} \exp\left(-\frac{(\delta - (1 - \mu_t))^2}{2\sigma_t^2}\right) \end{aligned}$$

for  $\delta \geq 1 - \mu_t$ , where the last inequality holds by the tail probability of the standard normal distribution. By (27), we have

$$\frac{1}{2} \leq 1 - \bar{\tau}t \leq \mu_t \leq 1 - \frac{\bar{\tau}t}{2} \quad \text{and} \quad \sqrt{\bar{\tau}t} \leq \sigma_t \leq \sqrt{2\bar{\tau}t}$$

for any  $0 \leq t \leq (2\bar{\tau})^{-1}$ . Let  $\delta = 1 - \mu_t + 2\sigma_t\sqrt{\log(1/\sigma_t)}$ . Combining last display with (104), a simple calculation yields that

$$\begin{aligned} & \int_{\|\mathbf{x}\|_\infty \leq 1} \left| \int_{\|\mathbf{y}\|_\infty \leq 1} \{p_0(\mathbf{x}) - p_0(\mathbf{y})\} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} \right| d\mathbf{x} \\ & \leq K\sqrt{D}2^D \mu_t^{-D} \delta^{\beta\wedge 1} + KD\sqrt{D}2^{D+1+\beta\wedge 1} \mu_t^{-D} \exp\left(-\frac{(\delta - (1 - \mu_t))^2}{2\sigma_t^2}\right) \\ & \leq K\sqrt{D}2^{D+1} \left(\bar{\tau}t + 2\sqrt{2\bar{\tau}t \log(1/\sqrt{\bar{\tau}t})}\right)^{\beta\wedge 1} + KD\sqrt{D}2^{2D+1+\beta\wedge 1} (\sqrt{2\bar{\tau}t})^2 \\ & \leq D_1 \{t \log(1/t)\}^{\frac{\beta\wedge 1}{2}} \end{aligned} \quad (106)$$

for any  $0 \leq t \leq (2\bar{\tau})^{-1} \wedge 1$ , where  $D_1 = D_1(\beta, D, K, \bar{\tau}, \underline{\tau})$ .

For any  $\mathbf{x} \in \mathbb{R}^D$ , we have

$$\begin{aligned} 1 - \int_{\|\mathbf{y}\|_\infty \leq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} &= 1 - \mu_t^{-D} + \mu_t^{-D} - \int_{\|\mathbf{y}\|_\infty \leq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} \\ &= 1 - \mu_t^{-D} + \int_{\|\mathbf{y}\|_\infty \geq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y}, \end{aligned}$$

where the last equality holds by (105). A simple calculation yields that

$$|1 - \mu_t^{-D}| = \mu_t^{-D} |\mu_t^D - 1| = \mu_t^{-D} |1 - \mu_t| \sum_{k=0}^{D-1} \mu_t^k \leq D2^D |1 - \mu_t| \leq D2^D \bar{\tau}t$$

for any  $0 \leq t \leq (2\bar{\tau})^{-1}$ . For  $\|\mathbf{x}\|_\infty \leq \mu_t - 2\sigma_t\sqrt{\log(1/\sigma_t)}$  and  $\|\sigma_t\mathbf{z} + \mathbf{x}\|_\infty \geq \mu_t$ , we have  $\|\sigma_t\mathbf{z}\|_\infty \geq \|\sigma_t\mathbf{z} + \mathbf{x}\|_\infty - \|\mathbf{x}\|_\infty \geq 2\sigma_t\sqrt{\log(1/\sigma_t)}$ . Then,

$$\int_{\|\mathbf{y}\|_\infty \geq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} = \mu_t^{-D} \int_{\|\sigma_t\mathbf{z} + \mathbf{x}\|_\infty \geq \mu_t} \phi_1(\mathbf{z}) d\mathbf{z} \leq \mu_t^{-D} \int_{\|\mathbf{z}\|_\infty \geq 2\sqrt{\log(1/\sigma_t)}} \phi_1(\mathbf{z}) d\mathbf{z}.$$

By the tail probability of the standard normal distribution, the last display is bounded by

$$\mu_t^{-D} \sum_{i=1}^D \int_{|z_i| \geq 2\sqrt{\log(1/\sigma_t)}} \phi_1(\mathbf{z}) d\mathbf{z} \leq 2D\mu_t^{-D} \sigma_t^2 \leq 2^{D+2} D\bar{\tau}t$$

for any  $0 \leq t \leq (2\bar{\tau})^{-1} \wedge 1$ . Then,

$$\begin{aligned} & \int_{\|\mathbf{x}\|_\infty \leq 1} p_0(\mathbf{x}) \left| 1 - \int_{\|\mathbf{y}\|_\infty \leq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} \right| d\mathbf{x} \\ & \leq D2^D \bar{\tau}t + \int_{\|\mathbf{x}\|_\infty \leq 1} p_0(\mathbf{x}) \int_{\|\mathbf{y}\|_\infty \geq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} d\mathbf{x} \\ & \leq D2^D \bar{\tau}t + 2^{D+2} D\bar{\tau}t + \int_{\mu_t - 2\sigma_t\sqrt{\log(1/\sigma_t)} \leq \|\mathbf{x}\|_\infty \leq 1} p_0(\mathbf{x}) \int_{\|\mathbf{y}\|_\infty \geq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} d\mathbf{x}. \end{aligned}$$

A simple telescoping sum implies that

$$\begin{aligned}
 & 2^D - \left(2\mu_t - 4\sigma_t\sqrt{\log(1/\sigma_t)}\right)^D \\
 &= \left(2 - 2\mu_t + 4\sigma_t\sqrt{\log(1/\sigma_t)}\right) \sum_{k=0}^{D-1} 2^{D-1-k} \left(2\mu_t - 4\sigma_t\sqrt{\log(1/\sigma_t)}\right)^k \\
 &\leq \left(2\bar{\tau}t + 4\sqrt{2\bar{\tau}t\log(1/\sqrt{\bar{\tau}t})}\right) 2^{D-1}D
 \end{aligned}$$

for  $0 \leq t \leq D_2$ , where  $D_2 = D_2(\bar{\tau}, \underline{\tau})$  is a small enough constant so that  $D_2 \leq (2\bar{\tau})^{-1} \wedge 1$  and  $2\mu_t - 4\sigma_t\sqrt{\log(1/\sigma_t)} \leq 2$  for  $t \leq D_2$ . Combining (105) with the last two displays, we have

$$\begin{aligned}
 & \left| \int_{\|\mathbf{x}\|_\infty \leq 1} p_0(\mathbf{x}) \left| 1 - \int_{\|\mathbf{y}\|_\infty \leq 1} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} \right| d\mathbf{x} \right. \\
 & \leq D2^D \mu_t^{-D} \bar{\tau}t + 2^{D+2} D \bar{\tau}t + KD2^D \left( \bar{\tau}t + 2\sqrt{2\bar{\tau}t\log(1/\sqrt{\bar{\tau}t})} \right) \\
 & \leq D_3 \sqrt{t\log(1/t)}
 \end{aligned}$$

for  $0 \leq t \leq D_2$ , where  $D_3 = D_3(D, K, \bar{\tau}, \underline{\tau})$ . Combining (103) and (106) with the last display, we have

$$\int_{\|\mathbf{x}\|_\infty \leq 1} |p_0(\mathbf{x}) - p_t(\mathbf{x})| d\mathbf{x} \leq D_1 \{t\log(1/t)\}^{\frac{\beta \wedge 1}{2}} + D_3 \sqrt{t\log(1/t)} \quad (107)$$

for  $0 \leq t \leq D_2$ .

Note that

$$\int_{\|\mathbf{x}\|_\infty \geq 1} p_t(\mathbf{x}) d\mathbf{x} \leq \int_{\|\mathbf{x}\|_\infty \geq \mu_t + 2\sigma_t\sqrt{\log(1/\sigma_t)}} p_t(\mathbf{x}) d\mathbf{x} + \int_{1 \leq \|\mathbf{x}\|_\infty \leq \mu_t + 2\sigma_t\sqrt{\log(1/\sigma_t)}} p_t(\mathbf{x}) d\mathbf{x}$$

and we bound each term on the RHS. For  $\|\mathbf{x}\|_\infty \geq \mu_t + 2\sigma_t\sqrt{\log(1/\sigma_t)}$  and  $\|\mathbf{y}\|_\infty \leq 1$ , we have  $\|\mathbf{x} - \mu_t\mathbf{y}\|_\infty \geq \|\mathbf{x}\|_\infty - \mu_t\|\mathbf{y}\|_\infty \geq 2\sigma_t\sqrt{\log(1/\sigma_t)}$ .

Then,

$$\begin{aligned}
 & \int_{\|\mathbf{x}\|_\infty \geq \mu_t + 2\sigma_t\sqrt{\log(1/\sigma_t)}} p_t(\mathbf{x}) d\mathbf{x} = \int_{\|\mathbf{x}\|_\infty \geq \mu_t + 2\sigma_t\sqrt{\log(1/\sigma_t)}} \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
 &= \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \int_{\|\mathbf{x}\|_\infty \geq \mu_t + 2\sigma_t\sqrt{\log(1/\sigma_t)}} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{x} d\mathbf{y} \\
 &\leq \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \int_{\|\mathbf{x} - \mu_t\mathbf{y}\|_\infty \geq 2\sigma_t\sqrt{\log(1/\sigma_t)}} \phi_{\sigma_t}(\mathbf{x} - \mu_t\mathbf{y}) d\mathbf{x} d\mathbf{y} \\
 &= \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \int_{\|\mathbf{z}\|_\infty \geq 2\sqrt{\log(1/\sigma_t)}} \phi_1(\mathbf{z}) d\mathbf{z} d\mathbf{y} = \int_{\|\mathbf{z}\|_\infty \geq 2\sqrt{\log(1/\sigma_t)}} \phi_1(\mathbf{z}) d\mathbf{z} \\
 &\leq \sum_{i=1}^D \int_{|z_i| \geq 2\sqrt{\log(1/\sigma_t)}} \phi_1(\mathbf{z}) d\mathbf{z} \leq 2D\sigma_t^2 \leq 4D\bar{\tau}t, \quad \forall 0 \leq t \leq (2\bar{\tau})^{-1},
 \end{aligned}$$

where the third inequality holds by the tail probability of the standard normal distribution. A simple calculation yields that

$$\begin{aligned}
 & \int_{1 \leq \|\mathbf{x}\|_\infty \leq \mu_t + 2\sigma_t \sqrt{\log(1/\sigma_t)}} p_t(\mathbf{x}) d\mathbf{x} \\
 &= \int_{1 \leq \|\mathbf{x}\|_\infty \leq \mu_t + 2\sigma_t \sqrt{\log(1/\sigma_t)}} \int_{\|\mathbf{y}\|_\infty \leq 1} p_0(\mathbf{y}) \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} d\mathbf{x} \\
 &\leq \int_{1 \leq \|\mathbf{x}\|_\infty \leq \mu_t + 2\sigma_t \sqrt{\log(1/\sigma_t)}} K \int_{\mathbb{R}^D} \phi_{\sigma_t}(\mathbf{x} - \mu_t \mathbf{y}) d\mathbf{y} d\mathbf{x} = K \mu_t^{-D} \left| \left( 2\mu_t + 4\sigma_t \sqrt{\log(1/\sigma_t)} \right)^D - 2^D \right| \\
 &\leq K \mu_t^{-D} \left( |2\mu_t - 2| + 4\sigma_t \sqrt{\log(1/\sigma_t)} \right) \sum_{k=0}^{D-1} \left( 2\mu_t + 4\sigma_t \sqrt{\log(1/\sigma_t)} \right)^{D-1-k} 2^k \\
 &\leq K 2^D \left( 2\bar{\tau}t + 4\sqrt{2\bar{\tau}t \log(1/\sqrt{\bar{\tau}t})} \right) D 4^D
 \end{aligned}$$

for  $0 \leq t \leq D_4$ , where  $D_4 = D_4(\bar{\tau}, \underline{\tau})$  is a small enough constant so that  $D_4 \leq D_2$  and  $\mu_t + 2\sigma_t \sqrt{\log(1/\sigma_t)} \leq 2$  for  $t \leq D_4$ . Combining with the last two displays, we have

$$\int_{\|\mathbf{x}\|_\infty \geq 1} p_t(\mathbf{x}) d\mathbf{x} \leq D_5 \sqrt{t \log(1/t)}$$

for  $0 \leq t \leq D_4$ , where  $D_5 = D_5(D, K, \bar{\tau})$ . Therefore, combining (107) with the last display,

$$\begin{aligned}
 \int_{\mathbb{R}^D} |p_0(\mathbf{x}) - p_t(\mathbf{x})| d\mathbf{x} &= \int_{\|\mathbf{x}\|_\infty \leq 1} |p_0(\mathbf{x}) - p_t(\mathbf{x})| d\mathbf{x} + \int_{\|\mathbf{x}\|_\infty \geq 1} p_t(\mathbf{x}) d\mathbf{x} \\
 &\leq D_1 \{t \log(1/t)\}^{\frac{\beta \wedge 1}{2}} + D_3 \sqrt{t \log(1/t)} + D_5 \sqrt{t \log(1/t)} \leq D_6 \{t \log(1/t)\}^{\frac{\beta \wedge 1}{2}}
 \end{aligned}$$

where  $D_6 = D_1 + D_3 + D_5$ . The assertion follows by redefining the constants. ■

## C.2 Proof of Lemma 27

**Proof** For neural networks  $\mathbf{f}, \tilde{\mathbf{f}} \in \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$ , let  $\{W_l, \mathbf{b}_l\}_{l \in [L]}$  and  $\{\tilde{W}_l, \tilde{\mathbf{b}}_l\}_{l \in [L]}$  be the parameter matrices of  $\mathbf{f}$  and  $\tilde{\mathbf{f}}$ , respectively. For  $l \in [L-1]$ , let

$$\mathbf{f}_l(\cdot) = \rho \left( \sum_{j=1}^{m_l} R_l^{(j)} \left( W_l Q_l^{(j)} \cdot + \mathbf{b}_l \right) \right) \quad \text{and} \quad \tilde{\mathbf{f}}_l(\cdot) = \rho \left( \sum_{j=1}^{m_l} R_l^{(j)} \left( \tilde{W}_l Q_l^{(j)} \cdot + \tilde{\mathbf{b}}_l \right) \right).$$

Given  $\epsilon > 0$ , assume that all parameter values of  $\mathbf{f}$  and  $\tilde{\mathbf{f}}$  are at most  $\epsilon$  away from each other. Then,

$$\begin{aligned} \|\mathbf{f}_l(\mathbf{x}) - \mathbf{f}_l(\tilde{\mathbf{x}})\|_\infty &\leq \left\| \sum_{j=1}^{m_l} R_l^{(j)} W_l Q_l^{(j)} (\mathbf{x} - \tilde{\mathbf{x}}) \right\|_\infty \\ &\leq \sum_{j=1}^{m_l} \left\| W_l Q_l^{(j)} (\mathbf{x} - \tilde{\mathbf{x}}) \right\|_\infty \leq \sum_{j=1}^{m_l} \left\{ d_l \|W_l\|_\infty \cdot \left\| Q_l^{(j)} (\mathbf{x} - \tilde{\mathbf{x}}) \right\|_\infty \right\} \\ &\leq m_l d_l M \|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty, \quad l \in [L-1], \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^{d_l}. \end{aligned}$$

because for  $\mathbf{z} \in \mathbb{R}^{n_2}$ ,  $n_1, n_2 \in \mathbb{N}$ , we have  $\|W\mathbf{z}\|_\infty \leq n_2 \|W\|_\infty \|\mathbf{z}\|_\infty$  for any matrix  $W \in \mathbb{R}^{n_1 \times n_2}$  and  $\|Q\mathbf{z}\|_\infty = \|\mathbf{z}\|_\infty$  for any  $n_1 \times n_1$  permutation matrix  $Q$ . A simple calculation yields that

$$\begin{aligned} &\|(\mathbf{f}_{L-1} \circ \cdots \circ \mathbf{f}_l)(\mathbf{x}) - (\mathbf{f}_{L-1} \circ \cdots \circ \mathbf{f}_l)(\tilde{\mathbf{x}})\|_\infty \\ &\leq \left( \prod_{i=l}^{L-1} m_i d_i M \right) \|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty, \quad l \in [L-1], \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^{d_l}. \end{aligned} \tag{108}$$

Similarly, we have

$$\begin{aligned} \|\mathbf{f}_l(\mathbf{x}) - \tilde{\mathbf{f}}_l(\mathbf{x})\|_\infty &\leq \left\| \sum_{j=1}^{m_l} R_l^{(j)} \left( (W_l - \tilde{W}_l) Q_l^{(j)} \mathbf{x} + \mathbf{b}_l - \tilde{\mathbf{b}}_l \right) \right\|_\infty \\ &\leq \sum_{j=1}^{m_l} \left\| (W_l - \tilde{W}_l) Q_l^{(j)} \mathbf{x} + (\mathbf{b}_l - \tilde{\mathbf{b}}_l) \right\|_\infty \leq \sum_{j=1}^{m_l} \left\{ \|W_l - \tilde{W}_l\|_\infty \cdot \|Q_l^{(j)} \mathbf{x}\|_\infty + \|\mathbf{b}_l - \tilde{\mathbf{b}}_l\|_\infty \right\} \\ &\leq m_l \epsilon (1 + d_l \|\mathbf{x}\|_\infty) \leq m_l d_l \epsilon (1 + \|\mathbf{x}\|_\infty), \quad l \in [L-1], \mathbf{x} \in \mathbb{R}^{d_l}. \end{aligned}$$

Note also that

$$\|\tilde{\mathbf{f}}_l(\mathbf{x})\|_\infty \leq \sum_{i=1}^{m_l} \left\| R_l^{(i)} \left( \tilde{W}_l Q_l^{(i)} \mathbf{x} + \tilde{\mathbf{b}}_l \right) \right\|_\infty \leq m_l d_l M (\|\mathbf{x}\|_\infty + 1)$$

and

$$\begin{aligned} \left\| (\tilde{\mathbf{f}}_1 \circ \cdots \circ \tilde{\mathbf{f}}_1)(\mathbf{x}) \right\|_\infty &\leq \left( \prod_{i=1}^l m_i d_i M \right) \|\mathbf{x}\|_\infty + \sum_{k=0}^{l-1} \left( \prod_{i=k+1}^l m_i d_i M \right) \\ &\leq (\|\mathbf{x}\|_\infty + l) \prod_{i=1}^l \{m_i d_i (M \vee 1)\}. \end{aligned}$$

It follows that

$$\begin{aligned}
 & \left\| \left( \mathbf{f}_{l+1} \circ \tilde{\mathbf{f}}_l \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\mathbf{x}) - \left( \tilde{\mathbf{f}}_{l+1} \circ \tilde{\mathbf{f}}_l \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\mathbf{x}) \right\|_\infty \\
 & \leq m_{l+1} d_{l+1} \epsilon \left\{ 1 + \left\| \left( \tilde{\mathbf{f}}_l \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\mathbf{x}) \right\|_\infty \right\} \\
 & \leq m_{l+1} d_{l+1} \epsilon \left[ 1 + (\|\mathbf{x}\|_\infty + l) \prod_{i=1}^l \{m_i d_i (M \vee 1)\} \right] \\
 & \leq \epsilon (M \vee 1)^{-1} (\|\mathbf{x}\|_\infty + l + 1) \prod_{i=1}^{l+1} \{m_i d_i (M \vee 1)\}, \quad l \in [L-2], \mathbf{x} \in \mathbb{R}^{d_1}.
 \end{aligned} \tag{109}$$

Let

$$\begin{aligned}
 \mathbf{f}^{(l)}(\cdot) &= \left( \mathbf{f}_{L-1} \circ \cdots \circ \mathbf{f}_{l+1} \circ \tilde{\mathbf{f}}_l \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\cdot), \quad l \in [L-2] \\
 \mathbf{f}^{(0)}(\cdot) &= \left( \mathbf{f}_{L-1} \circ \cdots \circ \mathbf{f}_1 \right) (\cdot) \quad \text{and} \quad \mathbf{f}^{(L-1)}(\cdot) = \left( \tilde{\mathbf{f}}_{L-1} \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\cdot).
 \end{aligned}$$

Combining with (108) and (109), we have

$$\begin{aligned}
 & \left\| \mathbf{f}^{(l)}(\mathbf{x}) - \mathbf{f}^{(l+1)}(\mathbf{x}) \right\|_\infty \\
 &= \left\| \left( \mathbf{f}_{L-1} \circ \cdots \circ \mathbf{f}_{l+1} \circ \tilde{\mathbf{f}}_l \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\mathbf{x}) - \left( \mathbf{f}_{L-1} \circ \cdots \circ \mathbf{f}_{l+2} \circ \tilde{\mathbf{f}}_{l+1} \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\mathbf{x}) \right\|_\infty \\
 & \leq \epsilon \left( \prod_{i=l+2}^{L-1} m_i d_i M \right) (M \vee 1)^{-1} (\|\mathbf{x}\|_\infty + l + 1) \prod_{i=1}^{l+1} \{m_i d_i (M \vee 1)\} \\
 & \leq \epsilon (M \vee 1)^{-1} (\|\mathbf{x}\|_\infty + l + 1) \prod_{i=1}^{L-1} \{m_i d_i (M \vee 1)\}, \quad l \in [L-3], \mathbf{x} \in \mathbb{R}^{d_1}
 \end{aligned}$$

and

$$\begin{aligned}
 & \left\| \mathbf{f}^{(L-2)}(\mathbf{x}) - \mathbf{f}^{(L-1)}(\mathbf{x}) \right\|_\infty \\
 &= \left\| \left( \mathbf{f}_{L-1} \circ \tilde{\mathbf{f}}_{L-2} \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\mathbf{x}) - \left( \tilde{\mathbf{f}}_{L-1} \circ \cdots \circ \tilde{\mathbf{f}}_1 \right) (\mathbf{x}) \right\|_\infty \\
 & \leq m_{L-1} d_{L-1} \epsilon \left[ 1 + (\|\mathbf{x}\|_\infty + L - 2) \prod_{i=1}^{L-2} \{m_i d_i (M \vee 1)\} \right] \\
 & \leq \epsilon (M \vee 1)^{-1} (\|\mathbf{x}\|_\infty + L - 1) \prod_{i=1}^{L-1} \{m_i d_i (M \vee 1)\}, \quad \mathbf{x} \in \mathbb{R}^{d_1}.
 \end{aligned}$$

A simple calculation yields that

$$\begin{aligned}
 \left\| \mathbf{f}(\mathbf{x}) - \tilde{\mathbf{f}}(\mathbf{x}) \right\|_{\infty} &\leq \sum_{l=0}^{L-2} \left\| W_L \left( \mathbf{f}^{(l)}(\mathbf{x}) - \mathbf{f}^{(l+1)}(\mathbf{x}) \right) \right\|_{\infty} + \left\| \left( W_L - \tilde{W}_L \right) \mathbf{f}^{(L-1)}(\mathbf{x}) - \left( \mathbf{b}_L - \tilde{\mathbf{b}}_L \right) \right\|_{\infty} \\
 &\leq d_L \|W_L\|_{\infty} \sum_{l=0}^{L-2} \left\| \mathbf{f}^{(l)}(\mathbf{x}) - \mathbf{f}^{(l+1)}(\mathbf{x}) \right\|_{\infty} + d_L \left\| W_L - \tilde{W}_L \right\|_{\infty} \cdot \left\| \mathbf{f}^{(L-1)}(\mathbf{x}) \right\|_{\infty} + \left\| \mathbf{b}_L - \tilde{\mathbf{b}}_L \right\|_{\infty} \\
 &\leq \epsilon d_L M (M \vee 1)^{-1} \left\{ \sum_{l=0}^{L-2} (l+1 + \|\mathbf{x}\|_{\infty}) \right\} \prod_{i=1}^{L-1} \{m_i d_i (M \vee 1)\} \\
 &\quad + \epsilon d_L (\|\mathbf{x}\|_{\infty} + L - 1) \prod_{i=1}^{L-1} \{m_i d_i (M \vee 1)\} + \epsilon \\
 &\leq \epsilon d_L \left\{ \frac{L(L+1)}{2} + L\|\mathbf{x}\|_{\infty} + 2 \right\} \prod_{i=1}^{L-1} \{m_i d_i (M \vee 1)\}, \quad \mathbf{x} \in \mathbb{R}^{d_1}.
 \end{aligned}$$

For  $\mathbf{x} \in [-C, C]^{d_1}$ , the last display is bounded by

$$\epsilon d_L L (L + C + 3) \prod_{i=1}^{L-1} \{m_i d_i (M \vee 1)\} \stackrel{\text{def}}{=} \delta.$$

The total number of parameters in  $\mathbf{f}$  is  $T \stackrel{\text{def}}{=} \sum_{i=1}^L (d_i + 1) d_{i+1}$  and there are  $\binom{T}{s}$  combinations to pick  $s$  non-zero parameters. Since  $s \leq T \leq 2L \|\mathbf{d}\|_{\infty}^2$  and  $\binom{T}{s} \leq T^s \leq (2L \|\mathbf{d}\|_{\infty}^2)^s$ , we have

$$\begin{aligned}
 &N \left( \delta, \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}}), \|\cdot\|_{L^{\infty}[-C, C]^{d_1}} \right) \\
 &\leq \sum_{s_0=1}^s \binom{T}{s_0} N(\epsilon, [-M, M]^{s_0}, \|\cdot\|_{\infty}) \\
 &\leq s (2L \|\mathbf{d}\|_{\infty}^2)^s \left( \frac{2M}{\epsilon} \vee 1 \right)^s \\
 &\leq (2L \|\mathbf{d}\|_{\infty}^2)^{s+1} \left( \frac{2MLd_L (L + C + 3) \prod_{i=1}^{L-1} \{m_i d_i (M \vee 1)\}}{\delta} \vee 1 \right)^s.
 \end{aligned}$$

For  $\delta < 1$ , the last display is bounded by

$$\left( \frac{4L^2 \|\mathbf{d}\|_{\infty}^2 \{\|\mathbf{m}\|_{\infty} \|\mathbf{d}\|_{\infty} (M \vee 1)\}^L (L + C + 3)}{\delta} \right)^{s+1}.$$

The assertion follows by taking the logarithm. ■

### C.3 Proof of Lemma 28

**Proof** For any  $\mathbf{x} \in [-1, 1]^D$ , we have

$$\ell_{\mathbf{f}}(\mathbf{x}) \leq \int_{\underline{T}}^{\bar{T}} 2\mathbb{E} \left[ \|\mathbf{f}(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 \right] + \frac{2\mathbb{E}[\|\mathbf{Z}\|_2^2]}{\sigma_t^2} dt \leq \int_{\underline{T}}^{\bar{T}} \frac{2DF^2 + 2D}{\sigma_t^2} dt,$$

where the last inequality holds because  $\|\mathbf{f}(\mathbf{x}, t)\|_\infty \leq F\sigma_t^{-1}$ . Since  $\sigma_t \geq \sqrt{\underline{\tau}t}$  for all  $t \geq 0$  by (27), we have

$$|\ell_{\mathbf{f}}(\mathbf{x})| \leq \underline{\tau}^{-1}2D(F^2 + 1)(\log \bar{T} - \log \underline{T}). \quad (110)$$

Lemma 7 implies that there exists a constant  $C_{S,2} = C_{S,2}(D, K, \tau_1, \bar{\tau}, \underline{\tau}) > 0$  such that

$$\|\mathbf{f}_0(\mu_t \mathbf{x} + \sigma_t \mathbf{z}, t)\|_2 \leq \frac{C_{S,2}}{\sigma_t} (\|\mathbf{z}\|_\infty \vee 1)$$

for any  $\mathbf{x} \in [-1, 1]^D$  and  $\mathbf{z} \in \mathbb{R}^D$ . Then,

$$\begin{aligned} \ell_{\mathbf{f}_0}(\mathbf{x}) &\leq \int_{\underline{T}}^{\bar{T}} 2\mathbb{E} \left[ \|\mathbf{f}_0(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 \right] + \frac{2\mathbb{E}[\|\mathbf{Z}\|_2^2]}{\sigma_t^2} dt \\ &\leq \int_{\underline{T}}^{\bar{T}} \frac{2C_{S,2}^2 \mathbb{E}[(\|\mathbf{Z}\|_\infty \vee 1)^2] + 2D}{\sigma_t^2} dt. \end{aligned}$$

Since  $(\|\mathbf{z}\|_\infty \vee 1)^2 \leq (\|\mathbf{z}\|_\infty + 1)^2 \leq (\|\mathbf{z}\|_2 + 1)^2 \leq 2\|\mathbf{z}\|_2^2 + 2$ , the last display is bounded by

$$\int_{\underline{T}}^{\bar{T}} \frac{2C_{S,2}^2(2D + 2) + 2D}{\sigma_t^2} dt \leq \underline{\tau}^{-1} \{2C_{S,2}^2(2D + 2) + 2D\} (\log \bar{T} - \log \underline{T}).$$

Combining the last display with (110), we have

$$|\nu_{\mathbf{f}}(\mathbf{x})| = |\ell_{\mathbf{f}}(\mathbf{x}) - \ell_{\mathbf{f}_0}(\mathbf{x})| \leq \ell_{\mathbf{f}}(\mathbf{x}) + \ell_{\mathbf{f}_0}(\mathbf{x}) \leq D_1(F^2 \vee 1)(\log \bar{T} - \log \underline{T}),$$

where  $D_1 = D_1(D, \underline{\tau}, C_{S,2})$ . The first assertion follows by redefining the constant.

Simple calculation yields that

$$\begin{aligned} |\nu_{\mathbf{f}}(\mathbf{x})| &= |\ell_{\mathbf{f}}(\mathbf{x}) - \ell_{\mathbf{f}_0}(\mathbf{x})| = \left| \mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \left\| \mathbf{f}(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{\mathbf{Z}}{\sigma_t} \right\|_2^2 - \left\| \mathbf{f}_0(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{\mathbf{Z}}{\sigma_t} \right\|_2^2 dt \right] \right| \\ &= \left| \mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \{(\mathbf{f} - \mathbf{f}_0)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\}^\top \left\{ (\mathbf{f} + \mathbf{f}_0)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{2\mathbf{Z}}{\sigma_t} \right\} dt \right] \right| \\ &\leq \mathbb{E} \left[ \sqrt{\int_{\underline{T}}^{\bar{T}} \|(\mathbf{f} - \mathbf{f}_0)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 dt} \sqrt{\int_{\underline{T}}^{\bar{T}} \left\| (\mathbf{f} + \mathbf{f}_0)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{2\mathbf{Z}}{\sigma_t} \right\|_2^2 dt} \right] \\ &\leq \sqrt{\mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \|(\mathbf{f} - \mathbf{f}_0)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 dt \right]} \sqrt{\mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \left\| (\mathbf{f} + \mathbf{f}_0)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{2\mathbf{Z}}{\sigma_t} \right\|_2^2 dt \right]} \\ &\leq \sqrt{\mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \|(\mathbf{f} - \mathbf{f}_0)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 dt \right]} \sqrt{2\ell_{\mathbf{f}}(\mathbf{x}) + 2\ell_{\mathbf{f}_0}(\mathbf{x})}, \end{aligned}$$

where the first and second inequalities hold by the Cauchy-Schwarz inequality. Combining with the last two displays, the second assertion follows by

$$\begin{aligned} \mathbb{E} \left[ \{\nu_{\mathbf{f}}(\mathbf{X}_0)\}^2 \right] &\leq \mathbb{E} \left[ (2\ell_{\mathbf{f}}(\mathbf{X}_0) + 2\ell_{\mathbf{f}_0}(\mathbf{X}_0)) \int_{\underline{T}}^{\bar{T}} \|(\mathbf{f} - \mathbf{f}_0)(\mu_t \mathbf{X}_0 + \sigma_t \mathbf{Z}, t)\|_2^2 dt \right] \\ &\leq 2D_1(F^2 \vee 1)(\log \bar{T} - \log \underline{T}) \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t)\|_2^2 \right] dt. \end{aligned}$$

■

#### C.4 Proof of Proposition 29

**Proof** Let  $\mathcal{F}$  be the class of functions  $\mathbf{f} : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^D$  satisfying  $\|\mathbf{f}(\cdot, t)\|_{L^\infty(\mathbb{R}^D)} \leq F\sigma_t^{-1}$  for all  $t \in [\underline{T}, \bar{T}]$ . Let  $\mathcal{V} = \{\nu_{\mathbf{f}}(\cdot) : \mathbf{f} \in \mathcal{F}\}$ . For  $\nu \in \mathcal{V}$ , denote

$$R(\nu) = \int_{[-1,1]^D} \nu(\mathbf{x})p_0(\mathbf{x})d\mathbf{x} \quad \text{and} \quad \widehat{R}_n(\nu) = \frac{1}{n} \sum_{i=1}^n \nu(\mathbf{X}^i).$$

Moreover, let

$$\tilde{\nu} \in \underset{\nu \in \mathcal{V}}{\operatorname{argmin}} R(\nu) \quad \text{and} \quad \widehat{\nu} \in \underset{\nu \in \mathcal{V}}{\operatorname{argmin}} \widehat{R}_n(\nu).$$

Note

$$\begin{aligned} R(\widehat{\nu}) &= R(\widehat{\nu}) - \widehat{R}_n(\widehat{\nu}) + \widehat{R}_n(\widehat{\nu}) \\ &\leq R(\widehat{\nu}) - \widehat{R}_n(\widehat{\nu}) + \widehat{R}_n(\tilde{\nu}) \\ &= R(\tilde{\nu}) + \left\{ R(\widehat{\nu}) - \widehat{R}_n(\widehat{\nu}) \right\} + \left\{ \widehat{R}_n(\tilde{\nu}) - R(\tilde{\nu}) \right\}, \end{aligned} \tag{111}$$

where the inequality holds because  $\widehat{\nu}$  is the ERM estimator. We bound each bracket term on the RHS.

Let  $\{\nu_1, \dots, \nu_{N_0}\} \subseteq \mathcal{V}$  be a minimal  $\epsilon$ -covering of  $\mathcal{V}$  in  $\|\cdot\|_{L^\infty([-1,1]^D)}$ -norm. Then, there exists  $j_* \in \{1, \dots, N_0\}$  such that  $\|\widehat{\nu} - \nu_{j_*}\|_{L^\infty([-1,1]^D)} \leq \epsilon$ . A simple calculation yields that

$$|R(\widehat{\nu}) - \widehat{R}_n(\widehat{\nu})| \leq 2\epsilon + |R(\nu_{j_*}) - \widehat{R}_n(\nu_{j_*})|. \tag{112}$$

For any  $\nu \in \mathcal{V}$ , Lemma 28 implies that

$$|\nu(\mathbf{X}^i) - R(\nu)| \leq D_1 \quad \text{and} \quad \mathbb{E} \left[ \left\{ \nu(\mathbf{X}^i) - R(\nu) \right\}^2 \right] \leq D_1 R(\nu) \quad \forall i \in [n],$$

where  $D_1 = 2\widetilde{C}_{14}(F^2 \vee 1)(\log \bar{T} - \log \underline{T})$  and  $\widetilde{C}_{14} = \widetilde{C}_{14}(D, K, \tau_1, \bar{\tau}, \underline{T})$  is the constant in Lemma 28. Lemma 2.2.9 from van der Vaart and Wellner (1996), which is standard Bernstein's inequality for bounded random variables, implies that for any  $r \geq 0$  and  $\nu \in \mathcal{V}$ ,

$$\mathbb{P} \left( \left| R(\nu) - \widehat{R}_n(\nu) \right| \geq \frac{1}{n} \left( \frac{2D_1 r}{3} + \sqrt{2nD_1 R(\nu)r} \right) \right) \leq 2e^{-r}$$

because for any  $M, v, t, x \geq 0$  with  $x \geq 2Mt/3 + \sqrt{2vt}$ ,  $x^2/(2v + 2Mx/3) \geq t$ . For any  $\delta > 0$ ,  $\sqrt{2D_1 R(\nu)r/n} \leq \delta D_1 R(\nu) + r/(n\delta)$  because  $\sqrt{2D_1 R(\nu)r/n} = \sqrt{2\{\delta D_1 R(\nu)\}\{r/(n\delta)\}}$  and  $\sqrt{2xy} \leq x + y$  for any  $x, y \geq 0$ . Combining with the last two displays, we have

$$\mathbb{P} \left( \left| R(\nu) - \widehat{R}_n(\nu) \right| \geq \delta D_1 R(\nu) + \frac{r}{n} \left( \frac{2D_1}{3} + \frac{1}{\delta} \right) \right) \leq 2e^{-r}$$

for any  $\delta, r > 0$  and  $\nu \in \mathcal{V}$ . The union bound implies that

$$\mathbb{P} \left( \left| R(\nu_j) - \widehat{R}_n(\nu_j) \right| \geq \delta D_1 R(\nu_j) + \frac{r + \log N_0}{n} \left( \frac{2D_1}{3} + \frac{1}{\delta} \right) \text{ for some } j \in [N_0] \right) \leq 2e^{-r}$$

and moreover,

$$\mathbb{P} \left( \left| R(\nu_j) - \widehat{R}_n(\nu_j) \right| \leq \delta D_1 R(\nu_j) + \frac{r + \log N_0}{n} \left( \frac{2D_1}{3} + \frac{1}{\delta} \right) \text{ for all } j \in [N_0] \right) \geq 1 - 2e^{-r}$$

for any  $\delta > 0$  and  $r > 0$ . Then,

$$\begin{aligned} \mathbb{E} \left[ |R(\nu_{j_*}) - \widehat{R}_n(\nu_{j_*})| \right] &\leq \delta D_1 \mathbb{E}[R(\nu_{j_*})] + \frac{r + \log N_0}{n} \left( \frac{2D_1}{3} + \frac{1}{\delta} \right) + 2D_1 e^{-r} \\ &\leq \delta D_1 \epsilon + \delta D_1 \mathbb{E}[R(\widehat{\nu})] + \frac{r + \log N_0}{n} \left( \frac{2D_1}{3} + \frac{1}{\delta} \right) + 2D_1 e^{-r} \end{aligned}$$

for any  $\delta > 0$  and  $r > 0$ . With  $\delta = 1/(2D_1)$  and  $r = 2 \log(2n)$ , simple calculation yields that

$$\mathbb{E} \left[ |R(\nu_{j_*}) - \widehat{R}_n(\nu_{j_*})| \right] \leq \frac{\mathbb{E}[R(\widehat{\nu})]}{2} + \frac{8D_1(2 \log 2 + 2 \log n + \log N_0)}{3n} + \frac{D_1}{2n^2} + \frac{\epsilon}{2}.$$

Combining with (112), we have

$$\mathbb{E} \left[ |R(\widehat{\nu}) - \widehat{R}_n(\widehat{\nu})| \right] \leq \frac{\mathbb{E}[R(\widehat{\nu})]}{2} + \frac{8D_1(2 \log(2n) + \log N_0)}{3n} + \frac{D_1}{2n^2} + \frac{5\epsilon}{2}.$$

Using the same computation as above for  $\mathbb{E} \left[ |R(\widetilde{\nu}) - \widehat{R}_n(\widetilde{\nu})| \right]$ , we have

$$\mathbb{E} \left[ |R(\widetilde{\nu}) - \widehat{R}_n(\widetilde{\nu})| \right] \leq \frac{R(\widetilde{\nu})}{2} + \frac{8D_1(2 \log(2n) + \log N_0)}{3n} + \frac{D_1}{2n^2} + \frac{5\epsilon}{2}.$$

Combining (111) with the last two displays, a simple calculation yields that

$$\frac{\mathbb{E}[R(\widehat{\nu})]}{2} \leq \frac{3R(\widetilde{\nu})}{2} + \frac{16D_1(2 \log(2n) + \log N_0)}{3n} + \frac{D_1}{n^2} + 5\epsilon$$

and moreover,

$$\begin{aligned} &\int_{\mathcal{T}}^{\overline{\mathcal{T}}} \mathbb{E} \left[ \left\| \widehat{\mathbf{f}}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t) \right\|_2^2 \right] dt \\ &\leq 3 \inf_{\widehat{\mathbf{f}} \in \widehat{\mathcal{F}}} \int_{\mathcal{T}}^{\overline{\mathcal{T}}} \mathbb{E} \left[ \left\| \mathbf{f}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t) \right\|_2^2 \right] dt + \frac{32D_1(2 \log(2n) + \log N_0)}{3n} + \frac{2D_1}{n^2} + 10\epsilon, \end{aligned} \tag{113}$$

where  $\widehat{\nu} = \nu_{\widehat{\mathbf{f}}}$  for some  $\widehat{\mathbf{f}} \in \widehat{\mathcal{F}}$ .

Let  $\tilde{\epsilon} > 0$ , which will be specified later and  $C = (1 + 2\sqrt{\log(1/\tilde{\epsilon})})\sqrt{\bar{T}}$ . Consider functions  $\mathbf{f}_1, \mathbf{f}_2 \in \mathcal{F}$  such that  $\|\mathbf{f}_1(\cdot) - \mathbf{f}_2(\cdot)\|_{L^\infty([-C, C]^{D+1})} \leq \tilde{\epsilon}$ . Then,

$$\begin{aligned}
 |\nu_{\mathbf{f}_1}(\mathbf{x}) - \nu_{\mathbf{f}_2}(\mathbf{x})| &= |\ell_{\mathbf{f}_1}(\mathbf{x}) - \ell_{\mathbf{f}_2}(\mathbf{x})| \\
 &= \left| \mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \left\| \mathbf{f}_1(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{\mathbf{Z}}{\sigma_t} \right\|_2^2 - \left\| \mathbf{f}_2(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{\mathbf{Z}}{\sigma_t} \right\|_2^2 dt \right] \right| \\
 &= \left| \mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \{(\mathbf{f}_1 - \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\}^\top \left\{ (\mathbf{f}_1 + \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{2\mathbf{Z}}{\sigma_t} \right\} dt \right] \right| \\
 &\leq \mathbb{E} \left[ \sqrt{\int_{\underline{T}}^{\bar{T}} \|(\mathbf{f}_1 - \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 dt} \sqrt{\int_{\underline{T}}^{\bar{T}} \left\| (\mathbf{f}_1 + \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{2\mathbf{Z}}{\sigma_t} \right\|_2^2 dt} \right] \\
 &\leq \sqrt{\mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \|(\mathbf{f}_1 - \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 dt \right]} \sqrt{\mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \left\| (\mathbf{f}_1 + \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t) + \frac{2\mathbf{Z}}{\sigma_t} \right\|_2^2 dt \right]} \\
 &\leq \sqrt{\mathbb{E} \left[ \int_{\underline{T}}^{\bar{T}} \|(\mathbf{f}_1 - \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 dt \right]} \sqrt{2\ell_{\mathbf{f}_1}(\mathbf{x}) + 2\ell_{\mathbf{f}_2}(\mathbf{x})},
 \end{aligned} \tag{114}$$

where the first and second inequalities hold by the Cauchy-Schwarz inequality. Since  $\|\mathbf{f}_1(\mathbf{x}, t) - \mathbf{f}_2(\mathbf{x}, t)\|_2^2 \leq 2\|\mathbf{f}_1(\mathbf{x}, t)\|_2^2 + 2\|\mathbf{f}_2(\mathbf{x}, t)\|_2^2 \leq 4DF^2\sigma_t^{-2}$ , we have

$$\mathbb{E} \left[ \|(\mathbf{f}_1 - \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 \right] \leq D\tilde{\epsilon}^2 + 4DF^2\sigma_t^{-2}\mathbb{P}(\|\mu_t \mathbf{x} + \sigma_t \mathbf{Z}\|_\infty \geq C)$$

for any  $t \in [\underline{T}, \bar{T}]$ . Let  $\mathbf{Z} = (Z_1, \dots, Z_D)$  and  $\mathbf{x} = (x_1, \dots, x_D)$ . Simple calculation yields that

$$\begin{aligned}
 \mathbb{P}(\|\mu_t \mathbf{x} + \sigma_t \mathbf{Z}\|_\infty \geq C) &\leq \sum_{i=1}^D \mathbb{P}(|\mu_t x_i + \sigma_t Z_i| \geq C) \\
 &= \sum_{i=1}^D \left\{ \mathbb{P}(Z_i \geq \sigma_t^{-1}(C - \mu_t x_i)) + \mathbb{P}(Z_i \leq -\sigma_t^{-1}(C + \mu_t x_i)) \right\} \\
 &\leq 2 \sum_{i=1}^D \mathbb{P}\left(Z_i \geq 2\sqrt{\log(1/\tilde{\epsilon})}\right),
 \end{aligned}$$

where the last inequality holds because  $0 < \sigma_t \leq 1$  and  $\mu_t \in [-1, 1]$ . Combining with the tail probability of the standard normal distribution, we have

$$\mathbb{P}(\|\mu_t \mathbf{x} + \sigma_t \mathbf{Z}\|_\infty \geq C) \leq 2D\tilde{\epsilon}^2.$$

Since  $\sigma_t \geq \sqrt{\bar{T}t}$  for any  $t \geq 0$ , we have

$$\begin{aligned}
 \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \|(\mathbf{f}_1 - \mathbf{f}_2)(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 \right] dt &\leq \int_{\underline{T}}^{\bar{T}} D\tilde{\epsilon}^2 + 8D^2F^2\sigma_t^{-2}\tilde{\epsilon}^2 dt \\
 &\leq D\bar{T}\tilde{\epsilon}^2 + 8D^2F^2\underline{T}^{-1}\tilde{\epsilon}^2(\log \bar{T} - \log \underline{T}) \leq D_2 \{ \bar{T} + F^2(\log \bar{T} - \log \underline{T}) \} \tilde{\epsilon}^2,
 \end{aligned} \tag{115}$$

where  $D_2 = D_2(D, \underline{\tau})$ . For any  $\mathbf{x} \in [-1, 1]^D$  and  $\mathbf{f} \in \mathcal{F}$ , we have

$$\ell_{\mathbf{f}}(\mathbf{x}) \leq \int_{\underline{T}}^{\bar{T}} 2\mathbb{E} \left[ \|\mathbf{f}(\mu_t \mathbf{x} + \sigma_t \mathbf{Z}, t)\|_2^2 \right] + \frac{2\mathbb{E}[\|\mathbf{Z}\|_2^2]}{\sigma_t^2} dt \leq \int_{\underline{T}}^{\bar{T}} \frac{2DF^2 + 2D}{\sigma_t^2} dt,$$

where the last inequality holds because  $\|\mathbf{f}(\mathbf{x}, t)\|_{\infty} \leq F\sigma_t^{-1}$ . Moreover,

$$\|\ell_{\mathbf{f}}(\cdot)\|_{L^{\infty}([-1, 1]^D)} \leq \underline{\tau}^{-1} 2D(F^2 + 1)(\log \bar{T} - \log \underline{T}).$$

Combining (114) and (115) with the last display, we have

$$\begin{aligned} |\nu_{\mathbf{f}_1}(\mathbf{x}) - \nu_{\mathbf{f}_2}(\mathbf{x})| &\leq \sqrt{4D_2 D \underline{\tau}^{-1} \{\bar{T} + F^2(\log \bar{T} - \log \underline{T})\} (F^2 + 1)(\log \bar{T} - \log \underline{T}) \tilde{\epsilon}^2} \\ &\leq D_3(F + 1)^2 \left( \sqrt{\bar{T}} + \sqrt{\log \bar{T} - \log \underline{T}} \right) \left( \sqrt{\log \bar{T} - \log \underline{T}} \right) \tilde{\epsilon}, \end{aligned}$$

where  $D_3 = D_3(D_2, D, \underline{\tau})$ . Let  $\epsilon = D_3(F + 1)^2(\sqrt{\bar{T}} + \sqrt{\log \bar{T} - \log \underline{T}})(\sqrt{\log \bar{T} - \log \underline{T}})n^{-2}$ . Then,

$$N \left( \epsilon, \mathcal{V}, \|\cdot\|_{L^{\infty}([-1, 1]^D)} \right) \leq N \left( n^{-2}, \mathcal{F}, \|\cdot\|_{L^{\infty}([-C, C]^{D+1})} \right).$$

Combining with (113), we have

$$\begin{aligned} &\int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \left\| \widehat{\mathbf{f}}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t) \right\|_2^2 \right] dt \\ &\leq 3 \inf_{\mathbf{f} \in \mathcal{F}} \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t)\|_2^2 \right] dt \\ &\quad + \frac{32D_1 \left\{ 2\log(2n) + \log N \left( n^{-2}, \mathcal{F}, \|\cdot\|_{L^{\infty}([-C, C]^{D+1})} \right) \right\}}{3n} \\ &\quad + \frac{D_1 + 10D_3(F + 1)^2 \left( \sqrt{\bar{T}} + \sqrt{\log \bar{T} - \log \underline{T}} \right) \left( \sqrt{\log \bar{T} - \log \underline{T}} \right)}{n^2}. \end{aligned}$$

Since  $D_1 = 2\tilde{C}_{14}(F^2 \vee 1)(\log \bar{T} - \log \underline{T})$ , there exists a constant  $D_4 = D_4(\tilde{C}_{14}, D_3)$  such that

$$\begin{aligned} &\int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \left\| \widehat{\mathbf{f}}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t) \right\|_2^2 \right] dt \\ &\leq 3 \inf_{\mathbf{f} \in \mathcal{F}} \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \|\mathbf{f}(\mathbf{X}_t, t) - \mathbf{f}_0(\mathbf{X}_t, t)\|_2^2 \right] dt \\ &\quad + \frac{D_5 \left\{ \log(2n) + \log N \left( n^{-2}, \mathcal{F}, \|\cdot\|_{L^{\infty}([-C, C]^{D+1})} \right) \right\}}{n}, \end{aligned}$$

where

$$D_5 = D_4(F^2 \vee 1) \left( \sqrt{\bar{T}} + \sqrt{\log \bar{T} - \log \underline{T}} \right) \left( \sqrt{\log \bar{T} - \log \underline{T}} \right).$$

The assertion follows by redefining the constants. ■

### C.5 Proof of Theorem 3

In this subsection, we provide the proof of Theorem 3 with auxiliary lemmas. For two probability measures  $P$  and  $Q$  on  $\mathcal{X} \subseteq \mathbb{R}^D$ , the Kullback-Leibler (KL) divergence is defined as

$$\text{KL}(P, Q) = \begin{cases} \int_{\mathcal{X}} \log \frac{dP}{dQ} dP, & \text{if } P \ll Q \\ \infty, & \text{else.} \end{cases}$$

We often denote  $\text{KL}(P, Q)$  as  $\text{KL}(p, q)$ , where  $p$  and  $q$  are densities of  $P$  and  $Q$ , respectively. Hereafter,  $C = C(\text{all})$  means that  $C$  is a constant depending on  $(\beta, d, D, K, \tau_{\min}, \tau_{\max}, \tau_1, \tau_2, \bar{\tau}, \underline{\tau})$ .

*Proof of Theorem 3.*

Let  $\tilde{\tau}_{\min} = \tau_{\min}(2\beta+d)/d$  and  $\tilde{\tau}_{\max} = \tau_{\max}(2\beta+d)/d$ . Let  $C_3, C_4$  be the constants in Theorem 5 depending on  $(\beta, d, D, K, \tilde{\tau}_{\min}, \tilde{\tau}_{\max}, \tau_1, \tau_2, \bar{\tau}, \underline{\tau})$ . Then, by replacing  $m$  in Theorem 5 with  $n^{d/(2\beta+d)}$ ,  $\underline{T}$  with  $m^{-\tilde{\tau}_{\min}}$ , and  $\bar{T}$  with  $\tilde{\tau}_{\max} \log m$ , there exists a class of permutation matrices  $\mathcal{P}_{\mathbf{m}}$  and a class of weight-sharing neural networks  $\mathcal{F}_{\text{WSNN}} = \mathcal{F}_{\text{WSNN}}(L, \mathbf{d}, s, M, \mathcal{P}_{\mathbf{m}})$  with

$$\begin{aligned} L &\leq D_1(\log n)^6 \log \log n, & \|\mathbf{d}\|_{\infty} &\leq D_1 n^{\frac{d(D+1)}{2\beta+d}}, \\ s &\leq D_1 n^{\frac{d}{2\beta+d}} (\log n)^5 \log \log n, & M &\leq \exp(D_1 \{\log n\}^6), \\ \|\mathbf{m}\|_{\infty} &\leq D_1 n^{\frac{dD}{2\beta+d}} \end{aligned}$$

satisfying

$$\inf_{\mathbf{f} \in \mathcal{F}_{\text{WSNN}} \cap \mathcal{F}_{\infty}} \int_{\underline{T}}^{\bar{T}} \int_{\mathbb{R}^D} \|\mathbf{f}(\mathbf{x}, t) - \nabla \log p_t(\mathbf{x})\|_2^2 p_t(\mathbf{x}) \, d\mathbf{x} dt \leq D_1 n^{-\frac{2\beta}{2\beta+d}} (\log n)^{4D+4\beta+1}, \quad (116)$$

for every  $n \geq C_4^{(2\beta+d)/d}$ , where  $\underline{T} = n^{-\tau_{\min}}$ ,  $\bar{T} = \tau_{\max} \log n$ ,  $D_1 = D_1(\beta, d, D, C_3)$  and

$$\mathcal{F}_{\infty} = \left\{ \|\mathbf{f}(\cdot, t)\|_{L^{\infty}(\mathbb{R}^D)} \leq D_1 \sigma_t^{-1} \sqrt{\log n} \quad \forall t \in [\underline{T}, \bar{T}] \right\}.$$

Let  $\hat{\mathbf{f}}$  be an empirical risk minimizer over the class  $\mathcal{F}_{\text{WSNN}} \cap \mathcal{F}_{\infty}$ , defined as in (6). By the Triangle inequality, we have

$$\mathbb{E} \left[ d_{\text{TV}}(P_0, \hat{P}_{\underline{T}}) \right] \leq d_{\text{TV}}(P_0, P_{\underline{T}}) + \mathbb{E} \left[ d_{\text{TV}}(P_{\underline{T}}, \hat{P}_{\underline{T}}) \right]. \quad (117)$$

We proceed to control each term on the RHS separately.

Let  $\tilde{C}_{12} = \tilde{C}_{12}(\beta, D, K, \bar{\tau}, \underline{\tau})$  and  $\tilde{C}_{13}(\bar{\tau}, \underline{\tau})$  be the constants in Lemma 26. Let  $D_2 = D_2(\beta, d, \tilde{C}_{13}, C_4)$  be a positive constant such that  $D_2 \geq C_4^{(2\beta+d)/d}$  and  $\underline{T} = n^{-\tau_{\min}} \leq \tilde{C}_{13}$  for every  $n \geq D_2$ . Then, Lemma 26 implies that

$$\begin{aligned} d_{\text{TV}}(P_0, P_{\underline{T}}) &= \frac{1}{2} \int_{\mathbb{R}^D} |p_0(\mathbf{x}) - p_{\underline{T}}(\mathbf{x})| \, d\mathbf{x} \\ &\leq 2^{-1} \tilde{C}_{12} \{\underline{T} \log(1/\underline{T})\}^{\frac{\beta \wedge 1}{2}} = 2^{-1} \tilde{C}_{12} \tau_{\min}^{(\beta \wedge 1)/2} n^{-\frac{\tau_{\min}(\beta \wedge 1)}{2}} (\log n)^{\frac{\beta \wedge 1}{2}}, \end{aligned}$$

for every  $n \geq D_2$ . Since  $\tau_{\min} \geq \frac{2\beta}{(2\beta+d)(\beta\wedge 1)}$ , the last display is bounded by

$$2^{-1} \tilde{C}_{12} \tau_{\min}^{(\beta\wedge 1)/2} n^{-\frac{\beta}{2\beta+d}} (\log n)^{\frac{\beta\wedge 1}{2}}. \quad (118)$$

Consider functions  $q_1, q_2 : \mathbb{R}^D \times [0, \bar{T} - \underline{T}] \rightarrow \mathbb{R}$  such that  $q_1(\mathbf{x}, t) = p_{\bar{T}-t}(\mathbf{x})$  and  $q_2(\mathbf{x}, t) = \hat{p}_{\bar{T}-t}(\mathbf{x})$ . Then, each  $q_1$  and  $q_2$  satisfy the corresponding well-known Fokker-Planck equation (Le Bris and Lions, 2008; Bogachev et al., 2022; Pavliotis, 2014) :

$$\begin{aligned} \frac{\partial}{\partial t} q_1(\mathbf{x}, t) &= - \sum_{i=1}^D \frac{\partial}{\partial x_i} [\mathbf{b}_1(\mathbf{x}, t) q_1(\mathbf{x}, t)] + \sum_{i=1}^D \sum_{j=1}^D \frac{\partial^2}{\partial x_i \partial x_j} [a_1(t) \delta_{ij} q_1(\mathbf{x}, t)] \\ \frac{\partial}{\partial t} q_2(\mathbf{x}, t) &= - \sum_{i=1}^D \frac{\partial}{\partial x_i} [\mathbf{b}_2(\mathbf{x}, t) q_2(\mathbf{x}, t)] + \sum_{i=1}^D \sum_{j=1}^D \frac{\partial^2}{\partial x_i \partial x_j} [a_2(t) \delta_{ij} q_2(\mathbf{x}, t)], \end{aligned}$$

where  $\delta_{ij}$  denotes the Kronecker delta and

$$\begin{aligned} \mathbf{b}_1(\mathbf{x}, t) &= \alpha_{\bar{T}-t} \mathbf{x} + 2\alpha_{\bar{T}-t} \nabla \log p_{\bar{T}-t}(\mathbf{x}), \quad a_1(t) = \alpha_{\bar{T}-t}, \\ \mathbf{b}_2(\mathbf{x}, t) &= \alpha_{\bar{T}-t} \mathbf{x} + 2\alpha_{\bar{T}-t} \hat{\mathbf{f}}(\mathbf{x}, \bar{T} - t), \quad a_2(t) = \alpha_{\bar{T}-t}. \end{aligned}$$

Following the Remark 2.3 of Bogachev et al. (2016), we have

$$\begin{aligned} d_{\text{TV}}(P_{\underline{T}}, \hat{P}_{\underline{T}}) &= d_{\text{TV}}(q_1(\cdot, \bar{T} - \underline{T}), q_2(\cdot, \bar{T} - \underline{T})) \\ &\leq d_{\text{TV}}(q_1(\cdot, 0), q_2(\cdot, 0)) + \left( \int_{\underline{T}}^{\bar{T}} \int_{\mathbb{R}^D} 4\alpha_t \left\| \hat{\mathbf{f}}(\mathbf{x}, t) - \nabla \log p_t(\mathbf{x}) \right\|_2^2 p_t(\mathbf{x}) d\mathbf{x} dt \right)^{1/2}. \end{aligned} \quad (119)$$

Recall that  $\hat{p}_{\bar{T}} = \phi_1$ . By Pinsker's inequality, we have

$$d_{\text{TV}}(q_1(\cdot, 0), q_2(\cdot, 0)) = d_{\text{TV}}(p_{\bar{T}}, \phi_1) \leq \sqrt{\text{KL}(p_{\bar{T}}, \phi_1) / 2}. \quad (120)$$

Since KL divergence is convex in its first argument, Jensen's inequality implies that

$$\text{KL}(p_{\bar{T}}, \phi_1) \leq \int_{\mathbb{R}^D} \text{KL}(\mathcal{N}(\mu_{\bar{T}} \mathbf{y}, \sigma_{\bar{T}} \mathbb{I}_D), \mathcal{N}(\mathbf{0}_D, \mathbb{I}_D)) dP_0(\mathbf{y}).$$

because  $p_{\bar{T}}(\cdot) = \int_{\mathbb{R}^D} \phi_{\sigma_{\bar{T}}}(\cdot - \mu_{\bar{T}} \mathbf{y}) dP_0(\mathbf{y})$ . KL divergence between two  $D$ -dimensional Gaussian random variables is known as

$$\begin{aligned} &\text{KL}(\mathcal{N}(\mu_1, \Sigma_1), \mathcal{N}(\mu_2, \Sigma_2)) \\ &= \frac{1}{2} \left[ \log \left( \frac{\det(\Sigma_2)}{\det(\Sigma_1)} \right) - D + (\mu_1 - \mu_2)^\top \Sigma_2^{-1} (\mu_1 - \mu_2) + \text{tr}(\Sigma_2^{-1} \Sigma_1) \right]. \end{aligned}$$

Using that, we have

$$\begin{aligned} \text{KL}(p_{\bar{T}}, \phi_1) &\leq \int_{\mathbb{R}^D} \frac{1}{2} (\mu_{\bar{T}}^2 \|\mathbf{y}\|_2^2 + D\sigma_{\bar{T}} - D - D \log \sigma_{\bar{T}}) dP_0(\mathbf{y}) \\ &= \frac{1}{2} (\mu_{\bar{T}}^2 \mathbb{E}_{P_0} [\|\mathbf{X}_0\|_2^2] + D\sigma_{\bar{T}} - D - D \log \sigma_{\bar{T}}) \\ &\leq \frac{D}{2} \left\{ \mu_{\bar{T}}^2 + \left| \sqrt{1 - \mu_{\bar{T}}^2} - 1 \right| + \left| \log(1 - \mu_{\bar{T}}^2) / 2 \right| \right\}, \end{aligned}$$

where the last inequality holds because  $\mathbb{E}[\|\mathbf{X}_0\|_2^2] \leq D$  and  $\mu_{\bar{T}}^2 + \sigma_{\bar{T}}^2 = 1$ . Since  $\mu_{\bar{T}} \leq \exp(-\underline{\tau}\bar{T})$  and  $|\log(1-x)| \leq x/(1-x)$  for  $0 < x < 1$ , the last display is bounded by

$$\frac{D}{2} \left\{ \mu_{\bar{T}}^2 + \frac{\mu_{\bar{T}}^2}{\sqrt{1-\mu_{\bar{T}}^2} + 1} + \frac{\mu_{\bar{T}}^2}{2(1-\mu_{\bar{T}}^2)} \right\}.$$

Note also that  $\mu_{\bar{T}}^2 \geq \exp(-2\bar{\tau}\bar{T}) = n^{-2\bar{\tau}\tau_{\max}}$  and  $\mu_{\bar{T}}^2 \leq \exp(-2\underline{\tau}\bar{T}) = n^{-2\underline{\tau}\tau_{\max}}$  by the definition. Let  $D_3 = D_3(\tau_{\max}, \bar{\tau}, D_2) > 0$  be a constant such that  $D_3 \geq D_2$  and  $n^{-2\bar{\tau}\tau_{\max}} \leq 1/2$  for every  $n \geq D_3$ . Then, the last display is further bounded by

$$\frac{5D\mu_{\bar{T}}^2}{4} \leq \left(\frac{5D}{4}\right) n^{-2\underline{\tau}\tau_{\max}} \leq \left(\frac{5D}{4}\right) n^{-\frac{2\beta}{2\beta+d}},$$

where the last inequality holds because  $\tau_{\max} \geq \frac{\beta}{\underline{\tau}(2\beta+d)}$ . Combining with (120), we have

$$d_{\text{TV}}(q_1(\cdot, 0), q_2(\cdot, 0)) = d_{\text{TV}}(p_{\bar{T}}, \phi_1) \leq \sqrt{5D/8} n^{-\frac{\beta}{2\beta+d}}, \quad \forall n \geq D_3. \quad (121)$$

Lemma 27 implies that there exists a constant  $D_4 = D_4(\beta, d, D, D_1)$  such that the metric entropy bound for  $\mathcal{F}$  follows by

$$\log N\left(n^{-2}, \mathcal{F}, \|\cdot\|_{L^\infty([-D_5, D_5]^{D+1})}\right) \leq D_4 n^{\frac{d}{2\beta+d}} (\log n)^{17} (\log \log n)^2, \quad (122)$$

where  $D_5 = (1 + 2\sqrt{2\log n}) \vee (\tau_{\max} \log n)$ . Let  $\tilde{C}_{14} = \tilde{C}_{14}(D, K, \tau_1, \bar{\tau}, \underline{\tau})$  be the constant in Proposition 29. Then, by replacing  $F$  in Proposition 29 with  $D_1\sqrt{\log n}$ , it follows that

$$\begin{aligned} & \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \left\| \widehat{\mathbf{f}}(\mathbf{X}_t, t) - \nabla \log p_t(X_t) \right\|_2^2 \right] dt \\ & \leq 3 \inf_{\mathbf{f} \in \mathcal{F} \cap \mathcal{F}_\infty} \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \left\| \mathbf{f}(\mathbf{X}_t, t) - \nabla \log p_t(\mathbf{X}_t) \right\|_2^2 \right] dt \\ & \quad + \frac{D_6(\log n)^2}{n} \left\{ \log N\left(n^{-2}, \mathcal{F} \cap \mathcal{F}_\infty, \|\cdot\|_{L^\infty([-D_5, D_5]^{D+1})}\right) + \log(2n) \right\}, \end{aligned}$$

where  $D_6 = D_6(\tau_{\max}, \tau_{\min}, D_1, \tilde{C}_{14})$ . Combining (116) and (122) with the last display, Jensen's inequality, we have

$$\begin{aligned} & \mathbb{E} \left[ \left\{ \int_{\underline{T}}^{\bar{T}} \left\| \widehat{\mathbf{f}}(\mathbf{X}_t, t) - \nabla \log p_t(\mathbf{X}_t) \right\|_2^2 dt \right\}^{1/2} \right] \\ & \leq \left\{ \int_{\underline{T}}^{\bar{T}} \mathbb{E} \left[ \left\| \widehat{\mathbf{f}}(\mathbf{X}_t, t) - \nabla \log p_t(\mathbf{X}_t) \right\|_2^2 \right] dt \right\}^{1/2} \\ & \leq D_7 n^{-\frac{\beta}{2\beta+d}} \left\{ (\log n)^{2D+2\beta+1} + (\log n)^{10} \right\}, \quad \forall n \geq D_3, \end{aligned}$$

where the first inequality holds by Jensen's inequality and  $D_7 = D_7(D_1, D_4, D_6)$ . Since  $\alpha_t \leq \bar{\tau}$  for all  $t \in [\underline{T}, \bar{T}]$ , combining (119) and (121) with the last display implies that

$$\mathbb{E} \left[ d_{\text{TV}} \left( P_{\underline{T}}, \widehat{P}_{\underline{T}} \right) \right] \leq D_8 n^{-\frac{\beta}{2\beta+d}} \left\{ (\log n)^{2D+2\beta+1} + (\log n)^{10} \right\}, \quad \forall n \geq D_3$$

where  $D_8 = D_8(D, \bar{\tau}, D_6)$ . Combining (117) and (118) with the last display, we have

$$\mathbb{E} \left[ d_{\text{TV}} \left( P_0, \widehat{P}_{\underline{T}} \right) \right] \leq D_9 n^{-\frac{\beta}{2\beta+d}} \left\{ (\log n)^{2D+2\beta+1} + (\log n)^{10} \right\}, \quad \forall n \geq D_3,$$

where  $D_9 = D_9(\beta, d, \tilde{C}_{12}, D_7)$ . The assertion follows by re-defining the constants. ■