A Functional-Space Mean-Field Theory of Partially-Trained Three-Layer Neural Networks

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Abstract

To understand the training dynamics of neural networks (NNs), prior studies have considered the infinite-width mean-field (MF) limit of two-layer NN, establishing theoretical guarantees of its convergence under gradient flow training as well as its approximation and generalization capabilities. In this work, we study the infinite-width limit of a type of three-layer NN model whose first layer is random and fixed. To define the limiting model rigorously, we generalize the MF theory of two-layer NNs by treating the neurons as belonging to functional spaces. Then, by writing the MF training dynamics as a kernel gradient flow with a time-varying kernel that remains positive-definite, we prove that its training loss in $L_2$ regression decays to zero at a linear rate. Furthermore, we define function spaces that include the solutions obtainable through the MF training dynamics and prove Rademacher complexity bounds for these spaces. Our theory accommodates different scaling choices of the model, resulting in two regimes of the MF limit that demonstrate distinctive behaviors while both exhibiting feature learning.

1 Introduction

Despite involving a non-convex optimization problem, the training of neural networks (NNs) can often succeed in practice under simple algorithms such as gradient descent (GD) and its variants. To understand this, prior studies have considered the training dynamics of NNs with large widths and their infinite-width limits. In particular, a series of works [15, 50, 65, 66, 70] studies shallow (a.k.a. two-layer, or 2L) NNs in the mean-field (MF) scaling — on an input space $\mathcal{X} \subseteq \mathbb{R}^d$, such a model maps any input $x \in \mathcal{X}$ to

$$
\frac{1}{m} \sum_{i=1}^{m} a_i \sigma(w_i^T \cdot x),
$$

where $m$ is the width of the hidden layer and $W = [W_{ij}]_{i \in [m], j \in [d]} = [w_1, \ldots, w_m]^T \in \mathbb{R}^{m \times d}$ and $a = [a_i]_{i \in [m]} \in \mathbb{R}^m$ are the parameters of the first and second layers, respectively, which are optimized during training. Such a model admits an integral representation and attains an infinite-width MF limit as $m \to \infty$ in the form of

$$
\int_{\mathbb{R} \times \mathbb{R}^d} a \sigma(w^T \cdot x) \mu(da, dh), \quad (1)
$$

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where \( \mu \in \mathcal{P}(\mathbb{R} \times \mathbb{R}^d) \). In the MF limit, the GD training dynamics (in continuous time) corresponds to a Wasserstein gradient flow (GF) followed by \( \mu \) in \( \mathcal{P}(\mathbb{R} \times \mathbb{R}^d) \), which can be proved to converge to global minimizers of the loss under suitable conditions [15, 50, 56, 65, 74]. Moreover, generalization and approximation guarantees can also be obtained for functions that exhibit an integral representation like (1) [5, 26], thus establishing a theoretical picture for wide two-layer NNs in the MF scaling that covers optimization, approximation, and generalization. However, the theory is limited in a few ways. First, despite several interesting attempts [2, 28, 54, 61, 71], an extension the theory to deeper NNs is not apparent. Second, the global convergence result of the training dynamics in the MF limit is asymptotic in both time and width — on one hand, no convergence rate of GD training is known in general settings, thus obstructing theoretical guarantees at any finite training time; on the other hand, though there have been efforts on quantifying the fluctuations between finite-width shallow NNs and the MF limit [10, 19, 51, 62, 69], global convergence guarantees that hold both in the MF limit and for models with a (large but) finite width have not been obtained.

In this work, we consider a type of partially-trained three-layer NN (P-3L NN) defined as:

\[
f^m_a(x; a, W) = \frac{1}{m_2} \sum_{i=1}^{m_2} a_i \sigma_2(h_i(x)),
\]

\[\forall i \in [m_2] : h_i(x) = \frac{1}{m_1^2} \sum_{j=1}^{m_1} W_{ij} \sigma_1(z_j \cdot x),\]  

(2)

where the pair \((m_1, m_2) =: m\) denotes the widths of the first and second hidden layers, respectively, \(\alpha\) is a scalar exponent, and \(\sigma_1, \sigma_2 : \mathbb{R} \to \mathbb{R}\) are the activation functions of the first and second hidden layers, respectively. \(W = [W_{ij}]_{i \in [m_2], j \in [m_1]} \in \mathbb{R}^{m_2 \times m_1}\) and \(a = [a_i]_{i \in [m_2]} \in \mathbb{R}^{m_2}\) are the parameters of the middle and last layers, respectively, and are both trained by GD. The first-layer parameters, \(z_1, ..., z_{m_1} \in \mathbb{R}^d\), are sampled randomly at initialization and untrained, hence the term “partially-trained”. For each \(i \in [m_2]\), we refer to the function \(h_i\) as the pre-activation function or feature map represented by the \(i\)th neuron in the second (or last) hidden layer.

When \(\alpha = 0\), if \(m_1 = m_2\) and the activation functions are 1-homogeneous (e.g., the ReLU function), the model (2) under i.i.d. random initialization of the parameters is equivalent to a three-layer NN under the Neural Tangent Kernel (NTK) scaling. In particular, as the widths tend to infinity, the model is known to approach a limit whose training dynamics is described by a kernel GF with a frozen kernel function called the NTK [37]. Through this observation, linear-rate convergence guarantees of the training loss [1, 12, 21, 22, 60, 80] as well as generalization bounds [3, 8, 25] have been proved for the model when the widths are large. However, the simplified analysis is a result of the large scaling of the model (i.e., \(\alpha\) is too small), under which the neurons barely move during training when the widths are large, indicating a lack of feature learning [17, 76]. For this reason, the NTK analysis does not fully explain the success of actual NNs, as shown by theoretical and empirical studies such as [31, 32, 33, 42, 73].

Alternatively, Chen et al. [11] consider the P-3L NN model with \(\alpha = \frac{1}{2}\) and both \(m_1\) and \(m_2\) large but finite, showing that not only does the model exhibit feature learning, but its training loss in \(L_2\) regression can also be proved to converge to zero at a linear rate. Then, natural questions are whether a well-defined limiting model exists as the widths \(m_1\) and \(m_2\) tend to infinity, and if so, whether it also admits both feature learning and convergence rate guarantees, as well as what space of functions it can explore. Note that if \(m_1\) is fixed while \(m_2\) tends to infinity, the model amounts to a two-layer NN in the MF scaling on top of a fixed embedding map from \(X\) to \(\mathbb{R}^{m_1}\) defined by the first layer, and hence an infinite-width limit can be derived analogously to the MF limit of two-layer NNs. However, this approach is no longer viable when \(m_1\) grows to infinity as well, and a new theory is called for to define the limiting model.
In this work, we develop a novel functional-space MF theory for the infinite-width limit of the P-3L model with $\alpha \geq \frac{1}{2}$. This will allow us to examine the training dynamics in the infinite-width limit rigorously, which can be written as a kernel GF with a time-varying kernel, and prove a linear-rate convergence guarantee of its training loss. We will see distinct behaviors of the infinite-width limit when choosing $\alpha = \frac{1}{2}$ versus $\alpha > \frac{1}{2}$, and for both regimes, we will define spaces of functions that are explored by the limiting model through training and prove generalization bounds by estimating their Rademacher complexity.

1.1 Related works

Convergence rate of shallow NNs in the MF scaling A number of studies have established the rate of convergence of the training of shallow NNs in the MF scaling, but typically only 1) under strong assumptions, 2) with modifications to the learning algorithm, or 3) in special tasks. As examples, Javanmard et al. [38] prove the linear-rate convergence of shallow NNs under GD under the assumption of displacement convexity, which is often too strong; Hu et al. [36], Nitanda et al. [58] and Chizat [13] prove that mean-field Langevin dynamics on shallow NNs can converge exponentially to global minimizers if the entropic regularization is strong enough; Chizat [14], Nitanda et al. [57], Rotskoff et al. [67], Wei et al. [73] and Oko et al. [59] propose other modifications to the GD algorithm under which the training loss of MF shallow NNs converge at an exponential or polynomial rate; Li et al. [43] prove that the a type of shallow NNs trained by truncated GD in a student-teacher setup with Gaussian inputs learns the target function in a polynomial number of iterations. In contrast with these works, we will study the training of shallow NNs in general $L_2$ regression tasks via vanilla GF without additional noise or regularization. Regarding negative results, Wojtowytsch and E [75] prove that if we train a shallow NN to fit a Lipschitz target function under population loss, the convergence rate cannot beat the curse of dimensionality. In comparison, we are interested in the empirical risk minimization (ERM) setting, where the loss function is the empirical risk evaluated on finitely many training data. The preceding work of Chen et al. [11] proves a linear-rate convergence guarantee for the $L_2$ training loss of the model defined by (2) when $\alpha = \frac{1}{2}$, which holds non-asymptotically in the width. The current work establishes the limit of this model as $m_1$ and $m_2$ jointly tend to infinity for a more general setting of $\alpha \geq \frac{1}{2}$. Then, we prove a similar linear-rate convergence rate guarantee for the limiting model through an insight that its training dynamics follows a kernel GF under kernel that is time-varying but positive-definite.

MF theory of multi-layer NNs The generalization of the MF limit of shallow NNs to multi-layer NNs is an intriguing and non-trivial task, and we refer the readers to Section 4.3 of [71] for an exposition of the challenges. However, a number of works have made such an effort. Nguyen [54] derives an MF limit of multi-layer NNs using heuristics of the symmetry among the neurons. By modeling the paths of weights while assuming that the first and last layers are untrained, Araujo et al. [2] derive a similar type of limit rigorously. Sirignano and Spiliopoulos [71] consider a different limit where the widths of the layers tend to infinity one at a time. Nguyen and Pham [55] and Pham and Nguyen [61] propose another MF limit of multi-layer NNs through an approach called neuronal embedding, and prove the global convergence of its training under the condition of bidirectional diversity. By characterizing a neuron through its feature maps on all the training data points, Fang et al. [28] derive an alternative dynamics for the infinite-width limits of multi-layer fully-connected NNs and Residual Networks (ResNets) [35] and prove that, when properly re-parameterized and regularized, the dynamics converges to global minimizers.

Though these approaches are highly interesting, they have a few limitations. First, these models adopt the “1/width” scaling in each layer (corresponding to setting $\alpha = 1$ in (2)), under which the
neurons tend to lose diversity when the widths tend to infinity, if the parameters are sampled i.i.d. at initialization and the model is deep [55]. This phenomenon calls for a reconsideration of the scaling of the model [46, 79]. In particular, Yang and Hu [77] propose an alternative maximum-update ($\mu P$) scaling, which allows both feature learning in the infinite-width limit [4] and a diversity of the neurons under i.i.d. initialization. However, neither convergence guarantees nor the associated function spaces have been derived for models in this scaling. Second, even though the global convergence of training has been proved under assumptions or reformulations of the training dynamics [28, 55, 61], no convergence rate has been derived. Third, largely due to the complicated nature of these models, not much insight has been gained regarding the function space corresponding to multi-layer fully-connected NNs. Meanwhile, E and Wojtowytsch [23] study a type of multi-layer models called neural trees and proposes a corresponding function space that generalizes the Barron space for shallow NNs, but its connection with the training of actual NNs is not apparent. Aside from fully-connected NNs, a few studies have also derived the continuous limits of deep ResNets [20, 26, 45], whose behavior is nevertheless quite different from fully-connected NNs with large widths in all layers. Finally, Korolev [40] studies the approximation theory of shallow NNs on Banach space inputs but does not consider training.

1.2 Our contributions

In this work, we derive an infinite-width MF-type limit of the P-3L NN model trained for $L_2$ regression by gradient flow (GF). By viewing the neurons in its second hidden layer through the functions they represent on the input domain, we characterize the limit as a probability measure on functional space, and hence the name functional-space MF limit. In particular,

- We prove the existence of the limit and the law of large numbers (LLN) as the widths tend to infinity. Unlike prior works [2, 28, 61, 71], our theory is applicable to not only the case $\alpha = 1$ in (2) but also the maximum-update scaling [77], which corresponds to setting $\alpha = \frac{1}{2}$;
- We prove that under i.i.d. initialization and with general activation functions, training loss converges to zero at a linear rate in the MF limit, under an insight that the training dynamics follows a kernel GF under a time-varying (and hence allowing feature learning, unlike in the NTK regime) kernel that remains positive definite;
- We derive function spaces that include the solutions learned by the P-3L model in the MF limit, which generalize the function spaces of shallow NNs defined in [5] and [26]. We then prove a generalization bound by estimating their Rademacher complexity;
- We perform numerical experiments on two synthetic tasks, whose results are consistent with 1) the existence of the infinite-width limit, 2) distinct behaviors between having $\alpha = \frac{1}{2}$ and $\alpha = 1$, and 3) differences with the NTK model as well as shallow NNs.

With these non-trivial and interesting properties, our functional-space MF theory of the P-3L NN can serve as a foundation of further studies of deep over-parameterized NNs.

2 Problem setup

2.1 Supervised $L_2$ regression and gradient flow (GF)

In this work, we focus on the supervised $L_2$ regression setup. Let $\mathcal{X} \subseteq \mathbb{R}^d$ be the input space, $\mathcal{Y} \subseteq \mathbb{R}$ be the output space, and $\mathcal{D}$ be an underlying joint distribution on $\mathcal{X} \times \mathcal{Y}$. The goal is to find a
function $f$ that achieves a low population risk $R_D(f)$, defined as
\[
R_D(f) = \frac{1}{2} \mathbb{E}_{(x,y) \sim D} [(f(x) - y)^2].
\]
In practice, instead of the true distribution $D$, we are typically given a training data set consisting of $n$ i.i.d. samples from $D$, $S = \{(x_1, y_1), \ldots, (x_n, y_n)\} \sim D^n$. Then, the strategy is to find a function that minimizes the empirical risk as a proxy, defined as
\[
\hat{R}_S(f) = \frac{1}{2n} \sum_{k=1}^{n} (f(x_k) - y_k)^2.
\]
To look for such a desired function, we parameterize the function by a P-3L NN and optimize its parameters using the empirical risk as the loss function, that is,
\[
L(a, W) = \hat{R}_S(f(\cdot; a, W)) = \frac{1}{2n} \sum_{k=1}^{n} (f^m(x_k; a, W) - y_k)^2.
\]
with $f^m$ defined in (2). For simplicity, we do not consider any regularization term. Computationally, we tackle the optimization problem by a combination of random initialization and GD training. First, we initialize each $a_{i,t}, W_{ij}$ and $z_j$ with values $a_{i,0}, W_{ij,0}$ and $z_{j,0}$, which are drawn randomly and independently from distributions $\rho_a, \rho_W$ and $\rho_z$, respectively. Next, for $t \geq 0$, we fix the value of each $z_j$ while evolving each $a_{i,t}$ and $W_{ij,t}$ by GD with respect to the loss function $L$. In this work, we limit our scope to studying the continuous-time version of GD, often called gradient flow (GF). Thus, if we use $\beta_0 \geq 0$ to represent the learning rate of $a_t = [a_{i,t}]_{i \in [m_2]}$ relative to $W_t = [W_{ij,t}]_{i \in [m_2], j \in [m_1]}$ and rescale the learning rate of $a_t$ by $m_2$ and that of the $W_t$ by $m_2 m_1^{-\alpha - 1}$, then each $a_{i,t}$ and $W_{ij,t}$ evolve in time according to
\[
\frac{d}{dt} a_{i,t} = -\frac{\beta_0}{\alpha} m_2 \frac{\partial L}{\partial a_{i,t}} (a_t, W_t) = -\frac{\beta_0}{\alpha} \frac{1}{n} \sum_{k=1}^{n} (f^m_t(x_k) - y_k) \sigma_2(h_{i,t}(x_k)) \tag{3}
\]
\[
\frac{d}{dt} W_{ij,t} = -m_2 m_1^{-\alpha - 1} \frac{\partial L}{\partial W_{ij,t}}(a_t, W_t)
= -\frac{\alpha_i}{m_1 - \alpha} \sum_{k=1}^{n} (f^m_t(x_k) - y_k) \sigma_2(h_{i,t}(x_k)) \sigma_1(z_j^\top \cdot x_k) \tag{4}
\]
Here we write $f^m_t = f^m_\alpha(a_t, W_t)$ and, for each $i \in [m_1]$, $h_{i,t} = \frac{1}{m_1} \sum_{j=1}^{m_1} W_{ij} \sigma_1(z_j^\top \cdot x)$, which then evolves in time according to
\[
\frac{d}{dt} h_{i,t}(x) = \frac{\alpha_i}{n} \sum_{k=1}^{n} (f^m_t(x_k) - y_k) \sigma_2(h_{i,t}(x_k)) \mathcal{G}^{m_1}(x_k, x) \tag{5}
\]
where for any $x, x' \in \mathcal{X}$, we define a kernel function $\mathcal{G}^{m_1}(x, x') = \frac{1}{m_1} \sum_{j=1}^{m_1} \sigma_1(z_j^\top \cdot x) \sigma_1(z_j^\top \cdot x')$, which has been called a random feature kernel or conjugate kernel [53, 64]. The evolution of the output function can be expressed as
\[
\frac{d}{dt} f^m_t(x) = \frac{1}{n} \sum_{k=1}^{n} (f^m_t(x_k) - y_k) \mathcal{K}^m_t(x_k, x) \tag{6}
\]
where for \( x, x' \in \mathcal{X} \), we define \( K^m(x, x') = \beta_a K^m_{a,t}(x, x') + K^m_W(x, x') \), with

\[
K^m_{a,t}(x, x') = \frac{1}{m^2_2} \sum_{i=1}^{m^2_2} \sigma_2(h_{i,t}(x)) \sigma_2(h_{i,t}(x')) ,
\]

\[
K^m_W(x, x') = \left( \frac{1}{m^2_2} \sum_{i=1}^{m^2_2} (a_{i,t})^2 \sigma_2'(h_{i,t}(x)) \sigma_2'(h_{i,t}(x')) \right) G^{m_1}(x, x') .
\]

This suggests that, because we rescaled the learning rates by \( m^2_2 \) in (3) and \( m^2_2 m'^{2a-1}_1 \) in (4), the contributions to the dynamics of \( f^m_t \) by the movements of \( a_t \) and \( W_t \) — corresponding to \( K^m_{a,t} \) and \( K^m_W \), respectively — both remain \( O(1) \) as \( m_1 \) and \( m_2 \) grow. In particular, when \( \alpha = \frac{1}{2} \), Chen et al. [11] show that up to a re-parameterization, this dynamics is consistent with the GD training of an Xavier-initialized NN under a constant learning rate.

It is then natural to ask if the dynamics of \( f^m_t \) governed by (6) admits any limit as \( m_1 \) and \( m_2 \) tend to infinity, and if so, what properties of the limiting dynamics can be deduced. To this end, we establish a functional-space MF theory in the next section.

### 2.2 Additional notations

We let \( \mathcal{X} \rightarrow \mathbb{R} \) denote the space of all real-valued functions on \( \mathbb{R} \), \( \mathcal{H} \) denote the reproducing kernel Hilbert space (RKHS) associated with the kernel function \( \mathcal{G} \), and \( \mathcal{C} = \mathcal{C}(\mathcal{X}, \mathbb{R}) \) denote the space of continuous functions on \( \mathcal{X} \). For any measurable space \( \Omega \), we let \( \mathcal{P}(\Omega) \) denote the set of all probability measures on \( \Omega \). We define \( \mathcal{G}_{\text{max}} = \sup_{x \in \mathcal{X}} \mathcal{G}(x, x) \) and \( y = [y_1, ..., y_n]^{\top} \in \mathbb{R}^n \). We let \( \text{Id}_n \) denote the \( n \times n \) identity matrix.

Let \( n' \in \mathbb{N}_+ \) and \( \{x'_1, ..., x'_{n'}\} \) be a subset of \( \mathcal{X} \). We let \( \mathcal{G}[x'_1, ..., x'_{n'}] \) and \( \mathcal{G}^{m_1}[x'_1, ..., x'_{n'}] \) denote the \( n' \times n' \) matrices defined by \( (\mathcal{G}[x'_1, ..., x'_{n'}])(kl) = \mathcal{G}(x'_k, x'_l) \) and \( (\mathcal{G}^{m_1}[x'_1, ..., x'_{n'}])(kl) = \mathcal{G}^{m_1}(x'_k, x'_l) \) for all \( k, l \in [n'] \), respectively. We define a finite-dimensional evaluation map \( e_{x'_1, ..., x'_{n'}} : (\mathcal{X} \rightarrow \mathbb{R}) \rightarrow \mathbb{R}^k \) that maps any real-valued function \( f \) on \( \mathcal{X} \) to \( [f(x'_1), ..., f(x'_{n'})] \in \mathbb{R}^k \). Then, we define a lifted map \( \hat{e}_{x'_1, ..., x'_{n'}} : \mathbb{R} \times (\mathcal{X} \rightarrow \mathbb{R}) \rightarrow \mathbb{R} \times \mathbb{R}^k \) that maps any \( a \in \mathbb{R} \) and any real-valued function \( f \) on \( \mathcal{X} \) to \( [a, e_{x'_1, ..., x'_{n'}}(f)]^{\top} \in \mathbb{R} \times \mathbb{R}^k \). We will then use \( (\hat{e}_{x'_1, ..., x'_{n'}})_\# \) to represent the push-forward map from \( \mathcal{P}(\mathbb{R} \times (\mathcal{X} \rightarrow \mathbb{R})) \) to \( \mathcal{P}(\mathbb{R} \times \mathbb{R}^k) \) induced by \( \hat{e}_{x'_1, ..., x'_{n'}} \), and let \( \mu_{t, [x'_1, ..., x'_{n'}]} \) and \( \mu^{m_1}_{t, [x'_1, ..., x'_{n'}]} \) denote \( (\hat{e}_{x'_1, ..., x'_{n'}})_\# \mu_t \) and \( (\hat{e}_{x'_1, ..., x'_{n'}})_\# \mu^{m_1}_t \) in \( \mathcal{P}(\mathbb{R} \times \mathbb{R}^k) \), respectively. In particular, with respect to the training data, we let \( G \) and \( G^{m_1} \) denote the \( n \times n \) matrices \( \mathcal{G}[x_1, ..., x_n] \) and \( \mathcal{G}^{m_1}[x_1, ..., x_n] \), respectively. We define \( G_{\text{min}} = \min_{k \in [n]} G_{kk} \) and let \( \lambda_{\text{min}}(G) \) denote the least eigenvalue of \( G \).

We also introduce the following shorthands for finite-dimensional evaluations with respect to the training data: \( e_\triangle = e_{x_1, ..., x_n}, \hat{e}_\triangle = \hat{e}_{x_1, ..., x_n}, \mu_\triangle = \mu_{t, [x_1, ..., x_n]} \) and \( \mu^{m_1}_t_\triangle = \mu^{m_1}_t_{[x_1, ..., x_n]} \).

In all the proofs within the appendix, we will write \( \sigma \) for \( \sigma^2 \) for simplicity.

### 3 A mean-field theory on functional space

#### 3.1 Integral representation on functional space

Suppose first that we fix \( m_1 \) while letting \( m_2 \) tend to infinity. Then, by the mean-field theory of a shallow NN, the limit can be described via a probability measure on \( \mathbb{R} \times \mathbb{R}^{m_1} \). Namely, if we consider the empirical measure on the parameter space, \( \frac{1}{m^2_2} \sum_{i=1}^{m^2_2} \int_{\mathcal{X}} \delta_{a_{i,t}}(da) \delta_{W_{i,t}}(dw) \in \mathcal{P}(\mathbb{R} \times \mathbb{R}^{m_1}) \), it converges weakly at each time to a MF measure as \( m_2 \rightarrow \infty \), which evolves in time according to a Wasserstein GF in the space \( \mathcal{P}(\mathbb{R} \times \mathbb{R}^{m_1}) \) [15, 50, 65, 66, 71]. When \( m_1 \) also tends to infinity,
however, it is not clear on what space the corresponding probability measure could be defined, and hence a more general theory is called for.

We begin by observing that, regardless of $m_1$, the pre-activation of each neuron in the second hidden layer, $h_i$, can always be viewed as a function on the input space $\mathcal{X}$, whose evolution in the functional space during training is governed by (5). Thus, instead of monitoring the movement of the weight vectors $\{(a_i,t, w_i,t)\}_{i \in [m_2]}$ directly, we can track the evolution of the ensemble of $\{(a_i,t, h_i,t)\}_{i \in [m_2]}$, by defining the following empirical measure on the space $\mathbb{R} \times (\mathcal{X} \to \mathbb{R})$,

$$
\mu^m_t(da, dh) = \frac{1}{m_2} \delta_{a,i,t}(da) \delta_{h_i,t}(dh),
$$

with which we can then write $f^m_t = f_{\mu^m_t}$, where we define, for any $\mu \in \mathcal{P}(\mathbb{R} \times (\mathcal{X} \to \mathbb{R}))$,

$$
f_\mu(x) = \int_{\mathbb{R} \times (\mathcal{X} \to \mathbb{R})} a \sigma_2(h(x)) \mu(da, dh).
$$

The dynamics of $a_t$ and $W_t$ under (3) and (5) induces an evolution of $\mu^m_t$ over time, which can be described by the push-forward of a time-varying transport map on $\mathbb{R} \times (\mathcal{X} \to \mathbb{R})$. Specifically, we can write $\mu^m_t = (\Theta^m_t) \# \mu^0_t$, where for $t \geq 0$, the map $\Theta^m_t : \mathbb{R} \times (\mathcal{X} \to \mathbb{R}) \to \mathbb{R} \times (\mathcal{X} \to \mathbb{R})$ can be decomposed as $\Theta^m_t(a,h) = [A^m_t(a,h), H^m_t(a,h)]$, with $A^m_t : \mathbb{R} \times (\mathcal{X} \to \mathbb{R}) \to \mathbb{R}$ and $H^m_t : \mathbb{R} \times (\mathcal{X} \to \mathbb{R}) \to (\mathcal{X} \to \mathbb{R})$ evolving according to the following equations:

$$
\frac{d}{dt} A^m_t(a,h) = \frac{1}{n} \sum_{k=1}^{m_2} (f^m_t(x_k) - y_k) \sigma_2(H^m_t(a,h)(x_k)),
$$

$$
\frac{d}{dt} H^m_t(a,h) = \frac{1}{n} A^m_t(a,h) \sum_{k=1}^{m_2} (f^m_t(x_k) - y_k) \sigma_2'(H^m_t(a,h)(x_k)) \mathcal{G}^{m_1}(x_k, \cdot),
$$

together with the initial condition

$$
A^m_0(a,h) = a, \quad H^m_0(a,h) = h.
$$

If $\mu^0_t$ converges to a limit $\mu_0$ as the widths $m_1$ and $m_2$ tend to infinity, it will be natural to consider a candidate for the infinite-width limit that we define as $\mu_t = (\Theta^m_t) \# \mu_0$, where for each $t \geq 0$, analogously to $\Theta^m_t$, the map $\Theta_t : \mathbb{R} \times (\mathcal{X} \to \mathbb{R}) \to \mathbb{R} \times (\mathcal{X} \to \mathbb{R})$ can be decomposed as $\Theta_t(a,h) = [A_t(a,h), H_t(a,h)]$, with $A_t : \mathbb{R} \times (\mathcal{X} \to \mathbb{R}) \to \mathbb{R}$ and $H_t : \mathbb{R} \times (\mathcal{X} \to \mathbb{R}) \to (\mathcal{X} \to \mathbb{R})$ evolving in time according to

$$
\frac{d}{dt} A_t(a,h) = \frac{1}{n} \sum_{k=1}^{m_2} (f_t(x_k) - y_k) \sigma_2(H_t(a,h)(x_k)),
$$

$$
\frac{d}{dt} H_t(a,h) = \frac{1}{n} A_t(a,h) \sum_{k=1}^{m_2} (f_t(x_k) - y_k) \sigma_2'(H_t(a,h)(x_k)) \mathcal{G}(x_k, \cdot),
$$

together with the initial condition

$$
A_0(a,h) = a, \quad H_0(a,h) = h.
$$

where we define $\mathcal{G}(x, x') = \lim_{m_1 \to \infty} \frac{1}{m_1} \sum_{j=1}^{m_1} \sigma_1(z_j^x \cdot x) \sigma(z_j^x \cdot x')$ and denote $f_t = f_{\mu_t}$. The dynamics governed by (9), (10) and (11) defines a measure-valued nonlinear transport partial differential equation (PDE) of McKean-Vlasov type [7, 49]. However, unlike the MF models of
interacting particle systems or shallow NNs, in our case, the evolving object $\mu_t$ is a probability measure on a functional space, which is, in principle, infinite-dimensional, and hence the prior results on the existence of the limit and the law of large numbers (LLN) do not immediately apply.

Hence, our initial goals will be to prove that there exist a pair of $\mu_t$ and $\Theta_t$ that satisfy this dynamics, and that $\mu_t$ is the limit of $\mu^m_t$ as $m_1, m_2 \to \infty$. As a first step, we want to gain a better understanding of the $\mu_t$ as defined above, starting with the simpler case $\alpha > \frac{1}{2}$.

### 3.2 Neurons in the reproducing kernel Hilbert space (RKHS): $\alpha > 1/2$

Suppose that $\alpha > \frac{1}{2}$ and the parameters are randomly sampled i.i.d. at initialization. Then as $m_1 \to \infty$, by the LLN, we see that for any $i \in [m_2]$ and any $x \in X$, $b_{i,0}(x)$ converges to zero almost surely. Thus, $\mu^m_0$ converges to the measure $\mu_0(da, dh) = \rho_0(da)\delta_0(dh)$, where $\delta_0$ is the singular measure at the constant-zero function. Rigorously, under the following assumptions on the smoothness of $\sigma_2$ and the choices of $\rho_0$, $\rho_W$ and $\rho_z$, we can prove that $\mu^m_0$ converges in 1-Wasserstein distance to $\mu_0$ under all finite-dimensional evaluations (as we define in Section 2.2):

**Assumption 1.** $\sigma_2$ is differentiable and its derivative $\sigma'_2$ is bounded and Lipschitz-continuous. Specifically, there exist $L_{\sigma_2}, L_{\sigma'_2} > 0$ such that $\forall u \in \mathbb{R}, |\sigma'_2(u)| \leq L_{\sigma_2}$ and $\sigma'_2$ is $L_{\sigma'_2}$-Lipschitz.

**Assumption 2.** $\rho_W = \mathcal{N}(0, 1)$, $\rho_0$ is sign-symmetric and compactly-supported and $\rho_z$ is sub-Gaussian.

**Lemma 3 (LLN at $t = 0$, $\alpha > \frac{1}{2}$).** Suppose $\alpha > \frac{1}{2}$ and Assumptions 1 and 2 hold. $\forall t \geq 0$, $\mu^m_0$ converges weakly in all finite-dimensional evaluations to $\mu_0 = \rho_0 \times \delta_0$ almost surely.

In particular, for any finite subset $\{x_1', ..., x_k'\} \subseteq X$ and $\forall \epsilon > 0, \exists K_1, K_2 > 0$ such that

$$\mathbb{P}\left(\mathcal{W}_1\left(\mu^m_0[x_1', ..., x_k'], \mu_0[x_1', ..., x_k']\right) > \epsilon\right) < O\left(e^{-K_1m_1} + e^{-K_2m_2}\right).$$

This lemma is proved in Appendix A.

Furthermore, for $t > 0$, we see that the right-hand side of (10) always belongs to the space of functions spanned linearly by $\{G(x_k, \cdot)\}_{k \in [n]}$, denoted by $\mathcal{H}_\Delta = \{h_{\lambda} = \sum_{k=1}^n \lambda_k G(x_k, \cdot) : \lambda \in \mathbb{R}^n\}$. In fact, it is a finite-dimensional subspace of a larger Hilbert space $\mathcal{H}$, which is the reproducing kernel Hilbert Space (RKHS) on $X$ associated with the kernel function $G$. Thus, for all $t \geq 0$, the measure $\mu_t$ is supported on $\mathbb{R} \times \mathcal{H}_\Delta \subseteq \mathbb{R} \times \mathcal{H}$, and hence $\Theta_t, A_t, H_t$ need only to be defined on $\mathbb{R} \times \mathcal{H}_\Delta$.

Abstractly, this allows us to interpret the model as a generalized shallow MF model where the first-layer parameters belong to a Hilbert space instead of the Euclidean space $\mathbb{R}^d$, and one can categorize it as a functional nonparametric model [29]. Moreover, the training dynamics corresponds to a Wasserstein gradient flow in $\mathcal{P}(\mathbb{R} \times \mathcal{H})$. Specifically, similarly to the Euclidean case [15], the Fréchet derivative of the loss can be defined as, for $a \in \mathbb{R}$, $h \in \mathcal{H}$,

$$\mathcal{L}'_{\mu}(a, h) = \sum_{k=1}^n \left(f_{\mu}(x_k) - y_k\right)\sigma_2(h(x_k)).$$

Recalling the reproducing property of $\mathcal{H}$ that $h(x) = \langle h, G(x, \cdot) \rangle_{\mathcal{H}}$, where $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is the inner product on $\mathcal{H}$, we are able to write $\nabla_h(h(x_k)) = G(x_k, \cdot) \in \mathcal{H}$ for $x \in X$. Hence, (9) and (10) can be equivalently written as

$$\frac{d}{dt} \Theta_t(a, h) = -\nabla \mathcal{L}'_{\mu}(\Theta_t^t(a, h)), \quad (13)$$

8
where for $\mu \in \mathcal{P}(\mathbb{R} \times \mathcal{H})$, $a \in \mathbb{R}$ and $h \in \mathcal{H}$,
\[
\nabla \mathcal{L}_t^\mu(\theta) = \left[ \frac{1}{n} \sum_{k=1}^n \left( f_\mu(x_k) - y_k \right) \sigma_2(h(x_k)) \right] \cdot \nabla \theta.
\]
Thus, (13) expresses a Wasserstein gradient flow in $\mathcal{P}(\mathbb{R} \times \mathcal{H})$, which is well-defined owning to the inner product structure of the Hilbert space $\mathcal{H}$. In comparison, while shallow NNs on Banach space inputs are defined in [40], no training scheme has been proposed.

To show the existence of $\mu_t$ as defined above, we rely on its equivalence with an alternative shallow MF model on an $n$-dimensional Euclidean space, as follows. Let $G \in \mathbb{R}^{n \times n}$ be defined by $G_{kl} = \mathcal{G}(x_k, x_l)$ for $k, l \in [n]$. First, we define a pair of linear maps $T : \mathbb{R}^n \to \mathcal{H}^\perp$ and $T^+ : (\mathcal{X} \to \mathbb{R}) \to \text{Ran}(G)$ as
\[
T(\lambda)(x) = h_{(G^+)\frac{1}{2}}(x), \quad T^+(h) = (G^+)\frac{1}{2} \cdot e_{\Delta}(h),
\]
where $G^+$ denotes the Moore-Penrose pseudo-inverse of $G$ and we use $e_{\Delta}$ as a shorthand for $e_{x_1, \ldots, x_n}$. We see that $T$ is a bijective map from $\text{Ran}(G) \subseteq \mathbb{R}^n$ to $\mathcal{H}^\perp$, with $T^+$ being its inverse map when restricted on $\mathcal{H}^\perp$. In fact, this is
\[
\|T(\lambda)\|_{\mathcal{H}} = (\lambda^T \cdot ((G^+)\frac{1}{2})^T \cdot G \cdot (G^+)\frac{1}{2} \cdot \lambda)^\frac{1}{2} = \|P_{\text{Ran}(G)}(\lambda)\|_2,
\]
and hence, $T$ is an isometry between $\text{Ran}(G)$ and $\mathcal{H}^\perp$. Moreover, for all $h_{\lambda} \in \mathcal{H}^\perp$,
\[
h_{\lambda}(x) = \sum_{k=1}^n \lambda_k \mathcal{G}(x_k, x) = (T^+(h_{\lambda}))^T \cdot \tilde{X}(x),
\]
where we define $\tilde{X} : \mathcal{X} \to \mathbb{R}^n$ as
\[
\tilde{X}(x) = \sum_{k=1}^n \mathcal{G}(x_k, x)((G^+)\frac{1}{2})_{k,:}.
\]
Therefore,
\[
f_t(x) = \int_{\mathbb{R} \times \mathcal{H}^\perp} a \sigma_2(h(x)) \mu_t(\text{d}a, \text{d}h) = \int_{\mathbb{R} \times \mathcal{H}^\perp} a \sigma_2((T^+(h))^T \cdot \tilde{X}(x)) \mu_t(\text{d}a, \text{d}h) = \int_{\mathbb{R} \times \mathbb{R}^n} a \sigma_2(\lambda^T \cdot X(x)) \nu_t(\text{d}a, \text{d}\lambda),
\]
where we define $\nu_t = (T^+)\#\mu_t$, with $T^+ : \mathbb{R} \times \mathcal{H}^\perp \to \mathbb{R} \times \text{Ran}(G)$ defined by $T^+(a, h) = [a, T^+(h)]$. For any $\nu \in \mathcal{P}(\mathbb{R} \times \mathbb{R}^n)$, letting $g_\nu$ denote the function on $\mathbb{R}^n$ defined by, $\forall \tilde{x} \in \mathbb{R}^n$,
\[
g_\nu(\tilde{x}) = \int_{\mathbb{R} \times \mathbb{R}^n} a \sigma(\lambda^T \cdot \tilde{x}) \nu(\text{d}a, \text{d}\lambda),
\]
then we can write $f_t(x) = g_\nu(\tilde{X}(x)) = g_t(\tilde{X}(x))$. Notably, $\nu_t$ can be viewed as a shallow MF model on $\mathbb{R}^n$ trained on an alternative set of training data, $\{(\tilde{x}_k, y_k)\}_{k \in [n]}$, where $\tilde{x}_k = \tilde{X}(x_k) = (G^+)\frac{1}{2}x_k$. In particular, $\nu_t$ is initialized as $\nu_0 = \rho_0 \times (\delta_0)^n$ and then follows a Wasserstein GF on $\mathcal{P}(\mathbb{R} \times \mathbb{R}^n)$ with respect to a loss $\mathcal{L}(\nu) = \frac{1}{n} \sum_{k=1}^n l(g_\nu(\tilde{x}_k), y_k)$. In other words, the model becomes equivalent to an $n$-dimensional shallow MF model applied to a transformed version of the input.
Hence, to show that $\mu_t$ exists, we can construct it from $\nu_t$, whose existence as a Wasserstein GF on finite-dimensional Euclidean space is known through prior literature [15, 70]. Specifically, it can be expressed as the push-forward by a time-varying transport map $\Psi^t$ on $\mathbb{R} \times \mathbb{R}^n, \nu_t = (\Psi^t)_# \nu_0$, where for $a \in \mathbb{R}$ and $\lambda \in \mathbb{R}^n$, $\Psi^t(a, \lambda) = [C_t(a, \lambda), \Lambda_t(a, \lambda)]$ with $C_t : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ and $\Lambda_t(a, \lambda) : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$, satisfying

$$\frac{d}{dt} C_t(a, \lambda) = \frac{1}{n} \sum_{k=1}^{n} (g_t(\bar{x}_k) - y_k) \sigma_2 (\Lambda_t(a, \lambda)^T \cdot \bar{x}_k),$$

$$\frac{d}{dt} \Lambda_t(a, \lambda) = \frac{1}{n} C_t(a, \lambda) \sum_{k=1}^{n} (g_t(\bar{x}_k) - y_k) \sigma_2 (\Lambda_t(a, \lambda)^T \cdot \bar{x}_k) \bar{x}_k,$$  \hspace{1cm} (16)

(17)

together with the initial conditions $C_0(a, \lambda) = a$ and $\Lambda_0(a, \lambda) = \lambda$. Then, if we define $A_t : \mathbb{R} \times \mathcal{H}_\Delta \to \mathbb{R}$ and $H_t : \mathbb{R} \times \mathcal{H}_\Delta \to \mathcal{H}_\Delta$ through

$$A_t(a, h) = C_t(a, T^+(h)),$$

$$H_t(a, h) = T \circ \Lambda_t(a, T^+(h)),$$  \hspace{1cm} (18)

(19)

it can be verified that they satisfy (9), (10) and (11). This allows us to conclude that,

**Lemma 4 (Existence of MF dynamics, $\alpha > \frac{1}{2}$).** Suppose $\alpha > \frac{1}{2}$ and Assumptions 1 holds. $\forall t \geq 0$ and $\forall \mu_0 \in \mathcal{P}(\mathbb{R} \times \mathcal{H}_\Delta), \exists \mu_t \in \mathcal{P}(\mathbb{R} \times \mathcal{H}_\Delta)$ and $\Theta_t : \mathbb{R} \times \mathcal{H}_\Delta \to \mathbb{R} \times \mathcal{H}_\Delta$ such that $\mu_t = (\Theta_t)_# \mu_0$, where $\mu_0 = \rho_a \times \delta_0$ and $\Theta_t = [A_t, H_t]$ satisfy (9), (10) and (11). In particular,

$$f_t(x) = g_t(\bar{X}(x)) = \int_{\mathbb{R} \times \mathbb{R}^n} a \sigma_2 (\lambda^T \cdot \bar{X}(x)) \nu_t(da, d\lambda),$$  \hspace{1cm} (20)

where $\nu_t = (\hat{T}^+)_# \mu_t = (\Psi_t)_# \nu_0$ with $\nu_0 = \rho_a \times (\delta_0)^n$.

3.3 Neurons as continuous functions: $\alpha = 1/2$

When $\alpha = \frac{1}{2}$, even at $t = 0$, the limiting MF measure $\mu_0$ is no longer supported within $\mathbb{R} \times \mathcal{H}$. In particular, The probability measure $\frac{1}{m} \sum_{i=1}^{m} \delta_{h_{t,i}}(dh)$ converges to the law of the sample paths of a Gaussian process with covariance function $\mathcal{G}$ [77], which, almost surely, do not belong to $\mathcal{H}$ [34]. This suggests that we need to consider the neurons as elements from a larger functional space than $\mathcal{H}$. The following result shows that the space of continuous functions on $\mathcal{X}$, denoted as $\mathcal{C} = \mathcal{C}(\mathcal{X}, \mathbb{R})$, suffices as such a choice.

**Lemma 5 (LLN at $t = 0, \alpha = \frac{1}{2}$).** Suppose Assumptions 1 and 2 hold. When $\alpha = \frac{1}{2}$, there exists a probability measure $\mu_0 = \rho_a \times \mathcal{G}(0, \mathcal{G})$ on $\mathbb{R} \times \mathcal{C}$ such that $\mu_0^n$ converges weakly in all finite-dimensional projections to $\mu_0 \in \mathcal{P}(\mathbb{R} \times \mathcal{C})$ almost surely, where $\mathcal{G}(0, \mathcal{G})$ denotes the law of the sample paths of a Gaussian process with mean zero and covariance function $\mathcal{G}$. In particular, for any finite subset $\{x_1', ..., x_k'\} \subseteq \mathcal{X}$ and $\forall \epsilon > 0, \exists K_1, K_2 > 0$ such that (12) holds.

This lemma is proved in Appendix B.

Like in the $\alpha > \frac{1}{2}$ case, the measure $\nu_t = (\hat{T}^+)_# \mu_t$ will still satisfy a Wasserstein GF in $\mathcal{P}(\mathbb{R} \times \mathbb{R}^n)$ under the loss $\hat{L}$, except for having a different initial condition $\nu_0 = \rho_a \times \mathcal{N}(0, \text{Id}_n)$ at $t = 0$. Nonetheless, as $\mu_t$ is no longer supported within $\mathcal{H}_\Delta$, the equivalence with the $n$-dimensional shallow MF model described by (15) no longer holds for all $x \in \mathcal{X}$, and hence the existence of $\mu_t$ is less straightforward to establish. However, as in the $\alpha > \frac{1}{2}$ case, the right-hand sides of (9) and (10)
depend on \(H_t(a, h)\) only through its function values on the training data, \(e_\triangle(h)\), or equivalently, its projection onto \(\mathcal{H}_\triangle\) defined as
\[
P_{\mathcal{H}_\triangle}(h) = T \circ T^+(h) = \sum_{k=1}^{n} \left(G^+ \cdot e_\triangle(h)\right)_k\mathcal{G}(x_k, \cdot).
\]

Moreover, for each \(k \in [n]\), since \((T^+(h))^\top \tilde{x}_k = (G^+ \cdot (G^+)^{\frac{1}{2}} \cdot e_\triangle(h))_k\) for any \(h \in \mathcal{C}\), it still holds that \(\forall k \in [n], f_t(x_k) = \int_{\mathbb{R} \times \mathcal{C}} \sigma_2(\left(T^+(h))^\top \tilde{x}(x_k)\right) \mu_t(da, dh) = g_t(\tilde{x}(x_k))\) as long as \(\mu_0, \alpha\) is supported within \(\mathbb{R} \times \text{Ran}(G)\), which is indeed implied by Lemma 5. In other words, the equivalence with the \(n\)-dimensional shallow MF model still holds on the training set. Thus, we can construct \(\mu_t\) from \(\nu_t = (\Psi_t)_{\#} \nu_0\) by defining \(A_t\) through (18) while defining \(H_t\) alternatively through
\[
H_t(a, h) = h + T \left(\Lambda_t(a, T^+(h)) - T^+(h)\right) = T \circ \Lambda_t(a, T^+(h)) + P_{\mathcal{H}_\triangle}^\perp(h),
\]
as an extension of (19) onto \(\mathbb{R} \times \mathcal{C}\), where for any \(h \in \mathcal{C}\), we define \(P_{\mathcal{H}_\triangle}^\perp(h) = h - P_{\mathcal{H}_\triangle}(h)\). It can then be verified that (9), (10) and (11) are satisfied. Therefore,

**Lemma 6 (Existence of MF dynamics, \(\alpha = \frac{1}{2}\)).** Suppose \(\alpha = \frac{1}{2}\) and Assumptions 1 holds. \(\forall t \geq 0\) and \(\forall \mu_0 \in \mathcal{P}(\mathbb{R} \times \mathcal{C})\) such that \(\mu_0, \alpha\) is supported within \(\mathbb{R} \times \text{Ran}(G)\), \(\exists \mu_t \in \mathcal{P}(\mathbb{R} \times \mathcal{C})\) and \(\Theta_t : \mathbb{R} \times \mathcal{C} \to \mathbb{R} \times \mathcal{C}\) such that \(\mu_t = (\Theta_t)_{\#} \mu_0\), where \(\mu_0 = \rho_0 \times \mathcal{G}(0, \mathcal{G})\) and \(\Theta_t = [A_t, H_t]\) satisfy (9), (10) and (11).

In particular, \(\forall x \in \mathcal{X}\), it holds that
\[
f_t(x) = \int_{\mathbb{R} \times \mathbb{R}^n} a E_{Z \sim \mathcal{N}(0, 1)} \left[\sigma_2(\tau_x Z + \sum_{k=1}^{n} ((G^+)^{\frac{1}{2}} \cdot \lambda)_k \mathcal{G}(x_k, x))\right] \nu_t(da, d\lambda)
\]
\[
= \int_{\mathbb{R} \times \mathbb{R}^n} a E_{Z \sim \mathcal{N}(0, 1)} \left[\sigma_2(\tau_x Z + \lambda^T \tilde{x}(x))\right] \nu_t(da, d\lambda),
\]
where \(\tau_x = \sqrt{\mathcal{G}(x, x) - \sum_{k,l=1}^{n} \mathcal{G}(x, x_k)\mathcal{G}(x, x_l)(G^+)_k,l} \geq 0\) and \(\nu_t = (\hat{T^+})_{\#} \mu_t = (\Psi_t)_{\#} \nu_0\) with \(\nu_0 = \rho_0 \times \mathcal{N}(0, I_d)\).

This lemma is proved in Appendix C. In particular, we see that \(\forall k \in [n], \tau_x x_k = 0\), and hence (20) remains true on the training data. Outside the training data, the additional term \(P_{\mathcal{H}_\triangle}^\perp(h)\) in (21) relative to (19) leads to the term \(\tau_x Z\) in (22), which one might interpret as adding an input-dependent uncertainty to the pre-activation of each neuron.

### 3.4 The law of large numbers

So far, we have shown the existence of \(\mu_t\) as a dynamics in the space of \(\mathcal{P}(\mathbb{R} \times \mathcal{C})\), which can be restricted to \(\mathcal{P}(\mathbb{R} \times \mathcal{H}_\triangle)\) when \(\alpha > \frac{1}{2}\). Next, we examine the convergence of \(f_t^m\) to \(f_t\) as \(m_1, m_2\) tend to infinity. While Lemmas 3 and 5 establish the convergence at \(t = 0\) under random initialization, for \(t > 0\), since the training dynamics introduce nonlinear interactions among the neurons, further arguments are necessary.

Classical studies of interacting particle systems rely on a propagation-of-chaos argument to bound the deviation between the finite-size system and its infinite-width limit through evolution using the Lipschitz-continuity of the evolution map [7]. This approach has been adapted to the showing that shallow NNs converge to the MF limit when the widths tend to infinity [15, 50, 65, 66, 70]. Here, we would like to adopt a similar approach, but are faced with the additional difficulty
that the probability measures are defined on an functional spaces rather than Euclidean space. To circumvent this issue, we again leverage the fact that the system can be alternatively represented by a transport dynamics of probability measures on finite-dimensional space, $\nu_t = (T^+)^\# \mu_t$, or equivalently, $\mu_{t,\Delta}$. First, we will prove the convergence of $\mu_{t,\Delta}$ to $\mu_{t,\Delta}$ as $m_1$ and $m_2$ tend to infinity. Specifically, if the activation function $\sigma_2$ is additionally assumed to be bounded, we can prove an upper bound on their 1-Wasserstein distance at time $t$ as a function of their 1-Wasserstein distance at time 0 as well as the deviation of $G^{m_1}$ from $G$:

**Assumption 7.** $\sigma_2$ is bounded. Specifically, $\exists M_{\sigma_2} > 0$ such that $\forall u \in \mathbb{R}, |\sigma_2(u)| \leq M_{\sigma_2}$.

**Lemma 8** (Quantitative propagation-of-chaos, I). Suppose Assumptions 1 and 7 hold and $\mu_t$ exists. Then for any $t \geq 0$, $\exists C_1(t) > 0$ such that

$$W_1(\mu_{t,\Delta}, \mu_{m,\Delta}) \leq C_1(t) \left( W_1(\mu_{0,\Delta}, \mu_{0,\Delta}) + \|G - G^{m_1}\|_2 \right). \quad (23)$$

This lemma is proved in Appendix D. Next, we extend the bound to any finite-dimensional evaluations of $\mu_t^m$ and $\mu_t$. Let $\{x'_1, ..., x'_{m'}\}$ be any finite subset of $\mathcal{X}$. We let $\mu_{t,\Delta} = (\hat{e}x'_1, ..., x'_{m'}) \# \mu_t$, $\mu_{t,\Delta}^m = (\hat{e}x'_1, ..., x'_{m'}) \# \mu_t^m$, $G_\Delta = \mathcal{G}[x_1, ..., x_n, x'_1, ..., x'_{m'}]$ and $G_{\Delta}^{m_1} := G^{m_1}[x_1, ..., x_n, x'_1, ..., x'_{m'}]$. Then,

**Lemma 9** (Quantitative propagation-of-chaos, II). Suppose Assumptions 1 and 7 hold and $\mu_t$ exists. For any $t \geq 0$, $\exists C_2(t) > 0$ such that

$$W_1(\mu_{t,\Delta}, \mu_{m,\Delta}) \leq C_2(t) \left( W_1(\mu_{0,\Delta}, \mu_{0,\Delta}) + W_1(\mu_{0,\Delta}, \mu_{0,\Delta}) + \|G_{\Delta} - G_{\Delta}^{m_1}\|_2 \right). \quad (24)$$

This lemma is proved in Appendix E.

Thus, combining Lemmas 3, 5, and 9 as well as concentration bounds of $G^{m_1}$ (Lemma 25), we see that $\forall t \geq 0$, $\epsilon > 0$, $\exists K_1, K_2 > 0$ such that

$$\mathbb{P} \left( W_1(\mu_{t,\Delta}, \mu_{t,\Delta}^m) > \epsilon \right) < O(e^{-K_1m_1} + e^{-K_2m_2}). \quad (25)$$

Hence, choosing $m' = 1$ and $x'_1 = x$, we are able to prove our main result on the MF limit:

**Theorem 10** (MF limit). Suppose Assumptions 1, 2 and 7 hold. Then $\mu_t = (\Theta_t) \# \mu_0$ exists, where $\Theta_t = [A_t, H_t]$ satisfy (9), (10) and (11), and $\mu_0 = \rho_0 \times \chi$, where $\chi = \delta_0$ if $\alpha > \frac{1}{2}$ or $\mathcal{G}P(0, \mathcal{G})$ if $\alpha = \frac{1}{2}$. Moreover, $\forall x \in \mathcal{X}, t \geq 0$, $f_t^m(x)$ converges almost surely as $m_1, m_2 \to \infty$ to $f_t(x) = f_{\mu_t}(x)$, which can be characterized by (20) and (22) when $\alpha > \frac{1}{2}$ and $\alpha = \frac{1}{2}$, respectively.

### 3.5 Extension to include the bias term

We can define a more general version of the P-3L NN model with the bias term included in the second hidden layer, as

$$f_t^m(x; a, b, W) = \frac{1}{m_2} \sum_{i=1}^{m_2} a_i \sigma_2(h_i(x)), \quad (26)$$

$$\forall i \in [m_2] : h_i(x) = b_i + \frac{1}{m_1} \sum_{j=1}^{m_1} W_{ij} \sigma_1(z_j^\top \cdot x),$$

where $b = [b_1, ..., b_{m_2}] \in \mathbb{R}^{m_2}$. During training, its dynamics is given by

$$\frac{d}{dt} b_{i,t} = -\frac{\beta b_{i,t}}{n} \sum_{k=1}^{n} \left( f_t^m(x_k) - y_k \right) \sigma_2'(h_{i,t}(x_k)), \quad (27)$$
where $\beta_b \geq 0$ denotes its learning rate relative to $W_t$. As $m_1, m_2 \to \infty$, the model can be described by a similar functional-space MF limit, namely, $\mu_t = (\Theta_t)_{\#}\mu_0$ with $\mu_0 = \rho_a \times \chi$. Compared to the bias-less case, (10) is replaced by
\[
\frac{d}{dt} H_t(a, h) = \frac{1}{n} A_t(a, h) \sum_{k=1}^{n} \left( f_t(x_k) - y_k \right) \sigma'(H_t(a, h)(x_k)) \left( \beta_b + G(x_k, \cdot) \right),
\]
and moreover, $\chi = \int_{\mathbb{R}} \delta_b \rho_b(db)$ if $\alpha > \frac{1}{2}$ and $\chi = \int_{\mathbb{R}} \mathcal{G}(b, \mathcal{G}) \rho_b(db)$ if $\alpha = \frac{1}{2}$, where for any $b \in \mathbb{R}$, $\delta_b$ denotes the singular measure at the constant function on $X$ with value $b$. The proof for the existence of the MF dynamics as well as the LLN is similar, and we omit it for consideration of space. We will also omit the bias term in the rest of this paper.

### 4 Kernel gradient flow and global convergence

In this section, we further investigate the dynamics of $f_t$ as a function on $X$. First, at initialization, there is $f_0(x) = (\int_{\mathbb{R}} a \rho_a(da)) (\int_{\mathbb{R}} \sigma(h(x)) \chi(dh))$, $\forall x \in X$. Hence, if $\rho_a$ is sign-symmetric (Assumption 2), then $f_0$ is identically 0 on $X$.

For $t \geq 0$, the evolution of the measure $\mu_t$ induces a dynamics of $f_t$ that can be expressed as a kernel gradient flow analogously to (6):
\[
\frac{d}{dt} f_t(x) = \frac{1}{n} \sum_{k=1}^{n} \left( f_t(x_k) - y_k \right) K_t(x_k, x),
\]
where for $x, x' \in X$, we define the kernel function $K_t(x, x') = \beta_b K_{a,t}(x, x') + K_{W,t}(x, x')$, with
\[
K_{a,t}(x, x') = \int_{\mathbb{R} \times C} \sigma(h(x)) \sigma(h(x')) \mu_t(da, dh),
\]
\[
K_{W,t}(x, x') = Q_t(x, x') \mathcal{G}(x, x'),
\]
where $Q_t(x, x') = \int_{\mathbb{R} \times C} a^2 \sigma'(h(x)) \sigma'(h(x')) \mu_t(da, dh)$.

The dynamics (27) can be regarded as a limit of the dynamics (6) as $m_1, m_2 \to \infty$, which is now well-defined through the theory developed in the previous section.

In the NTK regime (equivalent to $\alpha = 0$ if $\sigma$ is 1-homogeneous), the corresponding kernel function is static during training, which leads to a linearized training dynamics and excludes the possibility of feature learning [17]. In contrast, when $\alpha \geq \frac{1}{2}$, the kernel function $K_t$ changes over time as $\mu_t$ evolves during training. Inevitably, this complicates the convergence analyses compared to the NTK model, but we will show below that a linear-rate convergence guarantee can still be derived through a careful look at the kernel function.

#### 4.1 Linear-rate convergence with a time-varying kernel

To analyze the decay rate of the training loss, we define the $n \times n$ kernel matrix $K_t$ associated with the kernel function $K_t$ by $(K_t)_{kl} = K_t(x_k, x_l)$ for $k, l \in [n]$. Similarly, we define $n \times n$ matrices $K_{W,t}$ and $Q_t$ associated with $K_{W,t}$ and $Q_t$. It is easy to see that these matrices are symmetric and positive semi-definite. Then, from (27), the decay rate of the training loss can be computed as
\[
\frac{d}{dt} L_t = - \frac{1}{n^2} \sum_{k, l=1}^{n} (f_t(x_k) - y_k)(f_t(x_l) - y_l)(K_t)_{kl}.
\]
By the definition of the squared loss, letting $\lambda_{\min}()$ denote the minimum eigenvalue of a symmetric matrix, we obtain the following bound on the decay rate of the training loss, which is independent of the learning rate of the last layer, $\beta_a$:

$$
\frac{d}{dt} \mathcal{L}_t \leq -\frac{2}{n^2} \lambda_{\min}(K_t) \mathcal{L}_t \leq -\frac{2}{n^2} \lambda_{\min}(K_{W,t}) \mathcal{L}_t .
$$

(28)

Thus, if $\lambda_{\min}(K_{W,t})$ has a positive lower bound throughout training, (28) establishes a Polyak-Lojasiewicz (PL) condition \[44, 63\], through which one can prove that $\mathcal{L}_t$ converges to zero at a linear rate. Under the NTK limit mentioned above, since the kernel remains fixed during training, it suffices to prove that the kernel matrix is positive definite at initialization, which indeed holds in various settings \[21, 22\]. When $\alpha \geq \frac{1}{2}$, the kernel moves non-negligibly during training, and thus a uniform-in-time lower bound on $\lambda_{\min}(K_{W,t})$ is much less trivial. Nonetheless, we notice that the matrix $K_{W,t}$ can be written as the Hadamard (i.e. entry-wise) product of two matrices that are both positive semi-definite, $Q_t$ and $G$. Thus, to show the positive-definiteness of $K_{W,t}$, we can take advantage of Oppenheim’s inequality \[48\] to write

$$
\det(K_{W,t}) \geq \prod_{k=1}^{n} (Q_{tt})_{kk} \det(G) .
$$

(29)

On one hand, $G$ is independent of $t$ and often guaranteed to be positive definite, such as under the following mild assumptions on $\rho_z$, $\sigma_1$ and the training data \[21, 22\]:

**Assumption 11.** $\rho_z$ is $d$-dimensional standard Gaussian and $\sigma_1$ is either the ReLU function or analytic and non-polynomial.

**Assumption 12.** The training set $\{x_1, ..., x_n\}$ does not contain any pair of aligned vectors.

Therefore, we can conclude that $K_{W,t}$ is also positive definite as long as the diagonal entries of $Q_t$ has a positive lower bound that is uniform in time. This requires a more careful analysis of the dynamics, for which we require that the activation $\sigma_2$ satisfies:

**Assumption 13.** There exists an open interval $I = (I_l, I_r) \subseteq \mathbb{R}$ on which $\sigma_2$ is differentiable and $|\sigma_2'|$ is lower-bounded by some $K_{\sigma_2'} > 0$. If $\alpha > \frac{1}{2}$, we need to further assume that $0 \in I$.

The first part of this assumption is satisfied by most activation functions in practice, such as ReLU and tanh. The additional assumption $0 \in I$ for the case $\alpha > \frac{1}{2}$ is needed due to the bias term in the second hidden layer being omitted. If the bias term is added and randomly sampled from $\rho_b \in \mathcal{P}(\mathbb{R})$ at initialization, then this assumption can be replaced by $\rho_b(I) > 0$.

Together, we prove that the training loss converges to zero at a linear rate without requiring the kernel to be frozen during training:

**Theorem 14** (Linear-rate convergence of training loss). Suppose that Assumptions 1, 2, 11, 12 and 13 hold. Then there exist $\hat{a}$ and $r > 0$ such that if $\rho_a ([\hat{a}, \infty)) > 0$, then it holds that $\forall t \geq 0$,

$$
\mathcal{L}_t \leq \mathcal{L}_0 e^{-r\hat{a}^2 \lambda_{\min}(G)t} ,
$$

(30)

where $r$ depends on $\rho_a ([\hat{a}, \infty))$, $I$, $G_{\min}$, $\|y\|$, $M_{\sigma_2}$, $L_{\sigma_2}$ and $K_{\sigma_2'}$.

This theorem is proved in Appendix F. While non-asymptotic version of this result for the case $\alpha = \frac{1}{2}$ and $\beta_a = 0$ has been given in \[11\], our analysis offers novel insights via the kernel GF formulation.
5 Function spaces and generalization bound

In the following, we study the space of functions explored by the MF training dynamics. We will see that different spaces are obtained when \( \alpha > \frac{1}{2} \) versus \( \alpha = \frac{1}{2} \), and different techniques are used to estimate their complexity. For ease of exposition, the main text will present the theory under the assumption that \( \beta_a = 0 \) — thereby only considering the effect of training the middle layer — though the end result (Theorem 20) and its proof in the appendix will include the more general case of \( \beta_a \geq 0 \).

5.1 \( \alpha > 1/2 \)

Inspired by the function spaces of shallow NNs based on the integral representation \([5, 26]\), we define the following family of function spaces as their generalizations. Let \( \mathcal{U} \) be a normed vector space of real-valued functions on \( \mathcal{X} \) with norm \( \| \cdot \|_\mathcal{U} \), and let \( B(\mathcal{U}, \kappa) = \{ f \in \mathcal{U} : \| f \|_\mathcal{U} \leq \kappa \} \). Then, given a function \( f \) on \( \mathcal{X} \), we can define

\[
\gamma(f; \mathcal{U}) = \inf_{\mu} \int_{\mathbb{R} \times \mathcal{U}} |a| \| h \|_\mathcal{U} \mu(da, dh),
\]

where the infimum is taken over all \( \mu \in \mathcal{P}(\mathbb{R} \times \mathcal{U}) \) such that \( f(x) = \int_{\mathbb{R} \times \mathcal{U}} a \sigma_2(h(x)) \mu(da, dh) \). For \( \kappa \geq 0 \), we then use \( \mathcal{F}(\mathcal{U}, \kappa) \) to denote the space of all functions \( f \) on \( \mathcal{X} \) such that \( \gamma(f; \mathcal{U}) \leq \kappa \). We also define \( \mathcal{F}(\mathcal{U}) = \bigcup_{\kappa > 0} \mathcal{F}(\mathcal{U}, \kappa) \).

**Example 1.** If we choose \( \mathcal{U} = \mathbb{R}^d \) (and identify \( \mathbb{R}^d \) with the space of linear functions on \( \mathbb{R}^d \)), then \( \mathcal{F}(\mathbb{R}^d, \kappa) \) coincides with the Barron space \([26]\) and is equivalent to the variation-norm function space \([5]\) when the activation function is 1-homogeneous.

Meanwhile, choosing \( \mathcal{U} = \mathcal{H} \) allows us to define a function space for \( f_t \) when \( \alpha > \frac{1}{2} \), since we can estimate \( \gamma_{\mathcal{H}}(f_t) \) by the history of the loss values, \( \{ \mathcal{L}_s \}_{0 \leq s \leq t} \), via the following lemma:

**Lemma 15.** \( \forall t \geq 0, \int_{\mathbb{R} \times \mathcal{C}} \| H_t(a, h) - h \|_H \mu_0(da, dh) \leq \omega_t := \int_0^t \left( - \frac{d}{ds} \mathcal{L}_s \right)^{\frac{1}{2}} ds \). Under Assumptions 1 and 7, it also holds that \( \| H_t(a, h) - h \|_H \leq \sqrt{2} \mathcal{M}_{\sigma_2 \mathcal{L}_s a_1 \omega_t}, \forall (a, h) \in \text{supp}(\mu_0) \).

In particular, when \( \alpha > \frac{1}{2} \), Lemma 15 implies that \( f_t \in \mathcal{F}(\mathcal{H}, a_1 \omega_t) \). Moreover, when \( \sigma_2 \) is 1-homogeneous (e.g. ReLU, which unfortunately does not satisfy Assumption 1), we can control the Rademacher complexity of \( \mathcal{F}(\mathcal{U}, \kappa) \) by \( \kappa \) and the Rademacher complexity of the unit ball of \( \mathcal{U} \) via the following lemma, which is proved in Appendix H.

**Lemma 16.** If \( \sigma_2 \) is 1-homogeneous, then \( \text{Rad}_n(\mathcal{F}(\mathcal{U}, \kappa)) \leq L_\sigma \kappa \text{Rad}_n(B(\mathcal{U}, 1)) \).

Hence, via the Rademacher complexity of RKHS, we obtain the following as a corollary:

**Corollary 17.** If \( \sigma_2 \) is 1-homogeneous, then \( \text{Rad}_n(\mathcal{F}(\mathcal{H}, \kappa)) \leq L_\sigma (\mathcal{G}_\text{max})^{\frac{\kappa}{\sqrt{\pi}}} \).

5.2 \( \alpha = 1/2 \)

When \( \alpha = \frac{1}{2} \), there is no guarantee that \( \gamma(f_t; \mathcal{H}) < \infty \), even at \( t = 0 \). Although by choosing \( \mathcal{U} \) to be \( \mathcal{C} \) with a suitable norm, we could show that \( \gamma(f_t; \mathcal{C}) < \infty \) at finite \( t \geq 0 \), it will not be very helpful in deriving generalization guarantees since \( \mathcal{C} \) — and therefore \( \mathcal{F}(\mathcal{C}) \) — are too large to avoid the “curse of dimensionality”. Hence, we need a finer characterization of the space of functions that can be obtained from the dynamics. In particular, we want to limit our scope to those functions \( f_\mu \) that
evolve from a specific initial measure $\mu_0 = \mu_{\text{base}} \in \mathcal{P}(\mathbb{R} \times \mathcal{C})$ and control the deviation between $\mu_t$ and $\mu_{\text{base}}$ using Lemma 15.

To quantify the deviation, we define a type of Wasserstein-like extended metrics between probability measures on $\mathbb{R} \times \mathcal{C}$ as follows. Let $\mu, \mu'$ be two probability measures on $\mathbb{R} \times \mathcal{C}$, and let $\mathcal{J}(\mu, \mu')$ denote the space of probability measures on $\mathbb{R} \times \mathcal{C} \times \mathcal{C}$ that marginalize as $\mu$ and $\mu'$, in the sense that $\int_{\mathcal{C}} \pi(\cdot, \cdot, dh') = \mu$ and $\int_{\mathcal{C}} \pi(\cdot, dh, \cdot) = \mu'$. Then, inspired by Wasserstein distances between probability measures on metric spaces, we define

$$W_p(\mu, \mu'; \mathcal{U}) = \left( \inf_{\pi \in \mathcal{J}(\mu, \mu')} \| h - h' \|_{\mathcal{U}} \pi(da, dh, dh') \right)^{\frac{1}{p}},$$

for $p \geq 1$, and moreover,

$$W_\infty(\mu, \mu'; \mathcal{U}) = \inf_{\pi \in \mathcal{J}(\mu, \mu')} \sup_{(a, h', h) \in \text{supp}(\pi)} \| h - h' \|_{\mathcal{U}}.$$

Note that since the right-hand-sides may not be finite, these are extended metrics on $\mathcal{P}(\mathbb{R} \times \mathcal{C})$.

They allow us to define function spaces in the following way. Let $\mu_{\text{base}}$ be any probability measure on $\mathbb{R} \times \mathcal{C}$. Then, given any function $f$ on $\mathcal{X}$, for any $p \in [1, \infty]$, define

$$\gamma_p^\uparrow(f; \mathcal{U}, \mu_{\text{base}}) := \inf_{\mu} W_p(\mu, \mu_{\text{base}}; \mathcal{U}),$$

where the infimum is taken over all $\mu \in \mathcal{P}(\mathbb{R} \times \mathcal{C})$ such that $f(x) = \int_{\mathbb{R} \times \mathcal{C}} a \sigma_2(h(x)) \mu(da, dh)$. It is clear that for $1 \leq p \leq p' \leq \infty$, there is $\gamma_p^\uparrow(f; \mathcal{U}, \mu_{\text{base}}) \leq \gamma_{p'}^\uparrow(f; \mathcal{U}, \mu_{\text{base}})$ for any function $f$. Then, for any $\kappa \geq 0$, we can use $\mathcal{F}_p(\mathcal{U}, \mu_{\text{base}}, \kappa)$ to denote the space of all functions $f$ on $\mathcal{X}$ such that $\gamma_p^\uparrow(f; \mathcal{U}, \mu_{\text{base}}) \leq \kappa$. We also define $\mathcal{F}_p(\mathcal{U}, \mu_{\text{base}}) = \cup_{\kappa > 0} \mathcal{F}_p(\mathcal{U}, \mu_{\text{base}}, \kappa)$.

**Example 2.** Choosing $p \geq 2$ and $\mu_{\text{base}} = \rho_a \times \delta_0$ with $\rho_a$ compactly supported, it holds that $\mathcal{F}_p(\mathcal{U}, \rho_a \times \delta_0) = \mathcal{F}(\mathcal{U})$, thus recovering the function space corresponding to $\alpha > \frac{1}{2}$ if $\mathcal{U} = \mathcal{H}$.

More generally, choosing $\mathcal{U} = \mathcal{H}$ and $\mu_{\text{base}} = \mu_0$ allows us to define an appropriate function space for $f_t$ when $\alpha \geq \frac{1}{2}$. In particular, Lemma 15 implies that for any $t \geq 0$, $f_t \in \mathcal{F}_1(\mathcal{H}, \mu_0, \alpha_t \omega_t)$, and for $p \in [1, \infty]$, $f_t \in \mathcal{F}_p(\mathcal{H}, \mu_0, \kappa_t)$ with $\kappa_t = \sqrt{2} M_{\sigma} L_{\sigma} \alpha_t \omega_t$.

Moreover, the Rademacher complexity of $\mathcal{F}_p(\mathcal{H}, \mu_{\text{base}}, \kappa)$ can be controlled by $\kappa$ and the Rademacher complexity of the unit ball in $\mathcal{U}$, without homogeneity assumptions on $\sigma_2$:

**Lemma 18.** Assume that $\sigma_2$ is $L_{\sigma_2}$-Lipschitz and $\int_{\mathbb{R} \times \mathcal{C}} |a| \mu_{\text{base}}(da, dh) = \bar{a} < \infty$. Then

$$\text{Rad}_n(\mathcal{F}_p(\mathcal{H}, \mu_{\text{base}}, \kappa)) \leq L_{\sigma} \bar{a} \text{Rad}_n(\mathcal{B}(\mathcal{U}, \kappa)) \text{.}$$

This lemma is proved in Appendix I. As a corollary,

**Corollary 19.** $\text{Rad}_n(\mathcal{F}_\infty^\uparrow(\mathcal{H}, \mu_{\text{base}}, \kappa)) \leq L_{\sigma} \bar{a} G_{\max} \frac{\kappa}{\sqrt{n}}$.

In this way, with $\mu_{\text{base}} = \mu_0$, we are able to prove the following generalization bound for the MF P-3L model, which holds in the more general setting of $\beta_a \geq 0$:

**Theorem 20.** Let $\mathcal{D}$ be any distribution on $\mathcal{X} \times [-1, 1]$, and let $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ be i.i.d. sampled from $\mathcal{D}$. Let $f_t$ be the function learned through the MF dynamics at time $t \geq 0$, and let $\tilde{f}_t = ...$
min\{\max\{f_t, -1\}, 1\} be its truncation into \([-1, 1]\). Then for any \(\delta > 0\), with probability at least \(1 - \delta\) with respect to the sampling of \(S\),
\[
\mathcal{R}_D(\tilde{f}^t) \leq \mathcal{L}_t + 4C_1\left(\frac{\hat{\alpha}^2 + \beta_\alpha}{\sqrt{n}}\right) + \frac{\beta_\alpha M(\beta_\alpha, \hat{\alpha}, \omega_t)}{\sqrt{n}} + \sqrt{\frac{\log(\delta^{-1})}{2n}},
\]
(34)
where \(C_1 = \sqrt{2}(M_{\sigma_2})^3 + (M_{\sigma_2})^2 L_{\sigma_2}, M(\beta_\alpha, \hat{\alpha}, \omega_t) = C_2\omega_t \left(\left(\frac{\hat{\alpha}}{\alpha}\right)(\omega_t) + \beta_\alpha(\omega_t)^2 + \frac{\beta_\alpha^2}{\alpha}(\omega_t)^3\right)\), and
\[
\omega_t = \int_0^t \left(\frac{\alpha}{\sqrt{t}}\right)^{\frac{1}{2}} ds. \text{ In particular, if we choose } \beta_\alpha = 0, \text{ then this becomes}
\]
\[
\mathcal{R}_D(\tilde{f}^t) \leq \mathcal{L}_t + 4C_1\hat{\alpha}^2 \frac{\omega_t}{\sqrt{n}} + \sqrt{\frac{\log(\delta^{-1})}{2n}}.
\]
(35)

Remark 21. Recall that Proposition 14 implies that \(\forall t \geq 0\),
\[
\omega_t \leq \omega_\infty = \int_0^\infty \left(\mathcal{L}_0 e^{-r\hat{\alpha}^2 \lambda_{\min}(G)t}\right)^{\frac{1}{2}} dt = \frac{2(\mathcal{L}_0)^{\frac{1}{2}}}{r\hat{\alpha}^2 \lambda_{\min}}.
\]
Hence, when \(\beta_\alpha = 0\), the right-hand side of (35) converges to
\[
0 + \frac{8C_1(\mathcal{L}_0)^{\frac{1}{2}}}{r\lambda_{\min}(G)\sqrt{n}} + \sqrt{\frac{\log(\delta^{-1})}{2n}} \leq \frac{4\sqrt{2}C_1}{r\lambda_{\min}(G)\sqrt{n}} + \sqrt{\frac{\log(\delta^{-1})}{2n}}
\]
as \(t \to \infty\). This upper bound could be vacuous if \(\lambda_{\min}(G)\) decreases at a rate no slower than \(\frac{1}{\sqrt{n}}\), in which case the lower bound given in Proposition 14 on the global convergence rate via the least eigenvalue of the kernel matrix is potentially pessimistic.

Theorem 20 shall be viewed as giving an \textit{a posteriori} generalization bound — as opposed to \textit{a priori} ones [24] — due to the dependence on \(\omega_t\), which provides a complexity measure of the solution based purely on the training loss curve. It echoes the observation that when we train NNs to fit data with random labels, the convergence of training gets slower while the generalization performance becomes worse [78].

6 Numerical experiments

We perform numerical experiments on two datasets to demonstrate the existence of the infinite-width limits, the linear-rate convergence of training loss, the equivalence with the \(n\)-dimensional shallow MF dynamics as well as comparisons across different choices of \(\alpha\).

Tasks Both tasks are \(L_2\) regression tasks with inputs in \(\mathbb{R}^2\). The first one adopts a dataset considered in [16] and sets \(n = 18\). The second one has a training set with size \(n = 100\) sampled from four cocentric circles, whose labels depend alternately on the radius. This task is inspired by theoretical results on the advantage of deeper NNs in approximating and learning radial functions compared to shallow NNs [27, 68].

Models We consider three P-3L NN models — P-3L (\(\alpha = 1/2\)), P-3L (\(\alpha = 1\)) and P-3L (NTK) — all with \(m_1 = m_2 = m\). The P-3L (NTK) model uses the NTK parameterization and is equivalent to the P-3L model with \(\alpha = 0\) when \(\sigma = 1\)-homogeneous. In addition to the P-3L models, 2L is the shallow NN model with width \(m\), while \textbf{dim-}2L (\(N\)-init) and \textbf{dim-}2L (0-init) are the model
\[ g_t(\vec{X}(\cdot)) \text{ with } \nu_0 = \rho_a \times \mathcal{N}(0, \text{Id}_n) \text{ (corresponding to } \alpha = \frac{1}{2} \text{) and } \nu_0 = \rho_a \times (\delta_0)^n \text{ (corresponding to } \alpha = 1 \text{)}, respectively. We choose } \sigma_1 \text{ as ReLU so that the kernel function } \mathcal{G} \text{ can be computed analytically and used in the definition of the two dim-n 2L models. We consider choosing } \sigma_2 \text{ as tanh in task 1 and as either tanh or ReLU in task 2. The bias term in the (second) hidden layer is included and initialized to be zero, and we set } \beta_a = 0 \text{ and } \beta_b = 0.5.

Figure 1: Numerical results of various models on task 1. Row 1: curves of training (solid) and testing (dashed) errors versus number of GD steps. Row 2: distributions of the pre-activation values on a pair of data points in the (second) hidden layer, before (yellow) and after (magenta) training. Row 3: contour plots of the output function after training.

Results Figure 1 shows the empirical results on the first task where we set } \sigma_2 \text{ to be tanh. For } \text{P-3L NNs with } \alpha = 1 \text{ or } \frac{1}{2}, \text{ we see that the curves of training and testing losses are nearly uniform across different choices of } m, \text{ which is consistent with the existence of the infinite-width limits. Further, their training losses decay at a linear rate and the learned functions agree nicely with the corresponding } n \text{-dimensional shallow NN models (comparing Column 2 to Column 3 and Column 4 to Column 5). Under the NTK scaling, however, although it fits the training data well, the solution it learns performs poorly on the testing data. In fact, its distribution of pre-activation values in the second hidden layer barely moves during training, indicating a lack of feature learning [17].

Figures 2 and 3 show the empirical results on the second task in which } \sigma_2 \text{ is set to be tanh and ReLU, respectively. Note that the former case is covered by our theoretical results including Theorems 10, 14 and 20 while the latter case is not. We see that } \text{P-3L NNs with both } \alpha = \frac{1}{2} \text{ and } \alpha = 1 \text{ learn meaningful solutions whereas the shallow NN and the P-3L NN in the NTK regime fail to do so. In the case where } \sigma_2 \text{ is ReLU, } \text{P-3L (} \alpha = 1 \text{) also trains more slowly than } \text{P-3L (} \alpha = \frac{1}{2} \text{). Moreover, interestingly, we see that the long-time behavior of } \text{P-3L (} \alpha = 1 \text{) is distinct from that of dim-n 2L (0-init), seemingly at odds with (20). To further investigate this observation, for a fixed } t \text{ early in training, we plot the pre-activation values across neurons in the (second) hidden layer under different choices of the width } m. \text{ As shown in Figure 4, for the given } t, \text{ the distribution of pre-activation values in } \text{P-3L (} \alpha = 1 \text{) indeed converges to that in dim-n 2L (0-init) as } m \text{ grows,}
Figure 2: Numerical results of various models on task 2, where we choose $\sigma_2$ to be tanh. The plots have the same setting as in Figure 1.

Figure 3: Numerical results of various models on task 2, where we choose $\sigma_2$ to be ReLU. The plots have the same setting as in Figure 1.

thus reaffirming the existence of the infinite-width limit at finite time. Meanwhile, both dim-2L (0-init) and the infinite-width limit of P-3L ($\alpha = 1$) lack a diversity of the feature maps across the neurons in the (second) hidden layer, resulting in a qualitatively different behavior in training due to unbroken symmetry. Hence, we see that the two limits — the large-width limit ($m \to \infty$) and the long-time limit ($t \to \infty$) — do not interchange, indicating a limitation of the MF limit with $\alpha = 1$ as a model for finite-width P-3L NNs.
Finally, we test the models on variations of task 1 where the target labels of the training data are corrupted by additive Gaussian noise of different levels. We see from Figure 5 that as the noise variance increases, the training loss decays more slowly and the testing error becomes worse, which is compatible with what the generalization bound (35) suggests heuristically. Moreover, compared to the noiseless case, the distribution of pre-activation values in the second hidden layer evolves more significantly during training in the noisy case, which suggests, albeit non-quantitatively, that the solution learned in the noisy case likely has higher complexity as measured by (33).

Figure 4: (Second-)hidden-layer pre-activation values after 40 GD steps on task 2, where we choose $\sigma_2$ to be tanh. Each row corresponds to a different choice of $m$.

Figure 5: Results on noisy variations of task 1. **Row 1:** curves of training (solid) and testing (dashed) errors. **Rows 2 and 3:** (second-)hidden-layer pre-activation values in the *noiseless* and *noisy* settings before (yellow) and after (magenta) training.

7 Conclusions and limitations

In this work, we defined the infinite-width limit of a type of partially-trained three-layer NN by developing a functional-space MF theory. Through this theory, we proved a linear-rate convergence guarantee of the empirical loss for the limiting model. We then studied the functional spaces explored by the MF dynamics and presented a generalization bound through their Rademacher complexity. Our theory covers two different regimes of scaling the model output by its widths, which result in different behaviors through training despite both exhibiting feature learning, as we showed theoretically and empirically.

Our theory is limited in several ways. First, as we do not consider regularization terms, the final generalization bound in Theorem 20 is only a posteriori and possibly vacuous due to the convergence rate bound being pessimistic. Second, a comparison of the new function spaces with
the ones associated with shallow NNs is lacking. Third, the main theory needs boundedness and smoothness assumptions on the activation function of the second hidden layer, which therefore does not cover the ReLU function. Lastly, the P-3L NN model assumes that the parameters in the first layer are fixed, which is not often seen in practice. While some of these shortcomings appear to be still out of reach given the current techniques, the framework developed in this work could be a helpful stepping stone for further advances.

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A Proof of Lemma 3

Let \( \{x_1',...,x_n'\} \) be any finite subset of \( \mathcal{X} \). We define \( G' = G[x_1',...,x_n'] \) and \( G^{m_1} = G^{m_1}[x_1',...,x_n'] \). We denote \( e^* = e_{x_1',...,x_n'} \) and \( e^* = \hat{e}_{x_1',...,x_n'} \).

Recall that when \( \alpha > \frac{1}{2} \), \( e^*(\mu_0) = \rho_0 \times \delta_0 \). By the triangle inequality of 1-Wasserstein distance, there is

\[
\mathcal{W}_1(\hat{e}^*(\mu_0^m), \hat{e}^*(\mu_0)) = \mathcal{W}_1(\hat{e}^*(\mu_0^m), \rho_0 \times \delta_0) \\
\leq \mathcal{W}_1(\rho_0 \times \mathcal{N}(0, m_1^{1-2\alpha} G^{m_1}), \rho_0 \times \delta_0) \\
+ \mathcal{W}_1(\hat{e}^*(\mu_0^m), \mathcal{N}(0, m_1^{1-2\alpha} G^{m_1})).
\]

First, we examine the first term on the right-hand side. By the property of Wasserstein distances on product measures (e.g. Lemma 3 in [47]), we have

\[
\mathcal{W}_1(\rho_0 \times \mathcal{N}(0, m_1^{1-2\alpha} G^{m_1}), \rho_0 \times \delta_0) \\
\leq \mathcal{W}_1(\mathcal{N}(0, m_1^{1-2\alpha} G^{m_1}), \delta_0) \\
\leq \begin{pmatrix} \mathbb{E} \mathcal{Z} \in \mathcal{N}(0, G^{m_1}) \left\| m_1^{1/2-\alpha} \mathcal{Z} \right\|_2 \end{pmatrix}^{1/2} \\
\leq \frac{\mbox{Tr}(G^{m_1})}{m_1^{1/2-\alpha}} \leq \left( \frac{n G^{m_1}_{\max}^{m_1}}{m_1^{1/2}} \right)^{1/2}.
\]

For the second term, we see that, when conditioned on \( z_1,...,z_{m_1}, \{[a^0, h_0^0(x'_1),...,h_0^n(x'_n)]\}_{i\in[m_2]} \) is distributed i.i.d. across \( i \in [m_2] \) according to \( \rho_0 \times \mathcal{N}(0, m_1^{1-2\alpha} G^{m_1}) \). Hence, when conditioned on \( G^{m_1} \) (which is measurable with respect to \( z_1,...,z_{m_1} \)), \( e^*(\mu_0^m) \) has the same distribution as the empirical measure of \( m_2 \) i.i.d. samples from \( \rho_0^m \times \mathcal{N}(0, m_1^{1-2\alpha} G^{m_1}) \), which we denote by \( \nu(m_2) \in \mathcal{P}((\mathbb{R} \times \mathbb{R}^n)) \). Therefore, by conditioning on \( G^{m_1} \), we can leverage concentration inequalities in Wasserstein distance of empirical measures of i.i.d. samples:

**Lemma 22** (Adapted from [30], Theorem 2). Given a probability measure \( \nu \in \mathcal{P}(\mathbb{R}^d) \), let \( \nu(m) \) be the empirical measure of \( m \) i.i.d. samples from \( \nu \). If \( \exists \alpha > 1, \exists \gamma > 0 \) such that

\[
\mathcal{E}_{\alpha,\gamma}(\nu) := \int_{\mathbb{R}^d} e^{\gamma |x|^\alpha} \nu(dx) < \infty,
\]

then \( \forall m > 1, \forall u > 0, \)

\[
\mathbb{P}(\mathcal{W}_1(\nu(m), \nu) \geq u) \leq \begin{cases} C_1 e^{-C_2 m (u/\log(2+1/u))^2} I_{u \leq 1} + C_1 e^{-C_2 m u^\alpha} I_{u > 1}, & \text{if } d = 2 \\
C_1 e^{-C_2 m u^\alpha} I_{u \leq 1} + C_1 e^{-C_2 m u^\alpha} I_{u > 1}, & \text{if } d > 2,
\end{cases}
\]

where \( C_1 \) and \( C_2 \) depend only on \( d, \alpha, \gamma \) and \( \mathcal{E}_{\alpha,\gamma}(\nu) \).

In particular, choosing \( \nu = \rho_0 \times \mathcal{N}(0, m_1^{1-2\alpha} G^{m_1}) \), \( \alpha = 2 \), \( \gamma = \frac{1}{2 \lambda_{\max}(G^{m_1})} \), there is

\[
\mathcal{E}_{\alpha,\gamma}(\nu) = \int_{\mathbb{R}^d} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^{n'}} e^{\gamma \left(a^2 + m_1^{1-2\alpha}\|G^{m_1}\|_2 \cdot |u|^2\right)} e^{-\|u\|^2/2} du d\rho_0(da) \\
\leq e^{\gamma(a^0_{\max})^2} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^{n'}} e^{-m_1^{1-2\alpha} \lambda_{\max}(G^{m_1})\|u\|^2} du \\
\leq e^{\gamma(a^0_{\max})^2} \frac{2^{n'}}{(2\pi \cdot 2)^{n'}} \int_{\mathbb{R}^{n'}} e^{-\|u\|^2/2} du \\
\leq 2^{\frac{n'}{2}} e^{\gamma(a^0_{\max})^2/(2\lambda_{\max}(G^{m_1}))} < \infty.
\]
Therefore, applying Lemma 22, we have \( \forall u > 0, \exists C_1, C_2 > 0 \) such that

\[
\mathbb{P}\left( W_1(\hat{\epsilon}(\mu_0^m), \rho_a \times \mathcal{N}(0, m_1^{1-2\alpha}G^{m_1})) \geq u \right| G^{m_1}) = \mathbb{P}\left( W_1(\nu_{m_2}), \nu \geq u \right| G^{m_1}) \\
\leq C_1 e^{-C_2 u^{\max(n'+1,4)m_2}},
\]

where \( C_1 \) and \( C_2 \) depend only on \( n' \) and \( \lambda_{\max}(G^{m_1}) \). Furthermore, if we condition on the event that \( \| G^{m_1} - G' \|_2 < \Delta \) for some \( \Delta \in (0, \lambda_{\max}(G')) \), which is measurable with respect to \( G^{m_1} \), then by choosing \( \alpha = 2 \) and \( \gamma = \frac{1}{2(\lambda_{\max}(G') + \Delta)} \), we have \( \epsilon_{\alpha,\gamma}(\nu) \leq 2n' \epsilon(\alpha)^2/(2\lambda_{\max}(G^{m_1})) \leq 2n' \epsilon(\alpha)^2/\lambda_{\max}(G^{m_1}) < \infty \). Therefore, \( \forall u > 0, \exists C_1, C_2 > 0 \) depending only on \( n' \) and \( \lambda_{\max}(G') \) (instead of \( \lambda_{\max}(G^{m_1}) \)) such that,

\[
\mathbb{P}\left( W_1(\hat{\epsilon}(\mu_0^m), \rho_a \times \mathcal{N}(0, m_1^{1-2\alpha}G^{m_1})) \geq u \right| \| G^{m_1} - G' \|_2 < \Delta \) \leq C_1 e^{-C_2 u^{\max(n'+1,4)m_2}}.
\]

Thus, choosing \( \Delta = \lambda_{\max}(G') \), we know from Lemma 25 that

\[
\mathbb{P}\left( \| G^{m_1} - G' \|_2 \geq \Delta \right) < C_3(n')^2 e^{-C_4 \min(\Delta, C_5 \Delta^2)m_1}.
\]

Fix an \( \epsilon > 0 \). Conditioned on the event that \( \| G^{m_1} - G' \|_2 \leq \Delta = \lambda_{\max}(G') \), (37) implies that

\[
W_1(\rho_a \times \mathcal{N}(0, m_1^{1-2\alpha}G^{m_1}), \rho_a \times \delta_0) \leq \frac{1}{2} \epsilon,
\]

when \( m_1 \geq (\frac{8n'\Delta}{\epsilon^2})^{1/(2\alpha-1)} \). Thus, putting things together, if \( m_1 \geq (\frac{8n'\Delta}{\epsilon^2})^{1/(2\alpha-1)} \), then

\[
\begin{align*}
\mathbb{P}\left( W_1(\hat{\epsilon}(\mu_0^m), \hat{\epsilon}(\mu_0)) > \epsilon \right) \\
\leq \mathbb{P}\left( W_1(\hat{\epsilon}(\mu_0^m), \rho_a \times \delta_0) > \epsilon \right| \| G^{m_1} - G' \|_2 < \Delta \) + \mathbb{P}\left( \| G^{m_1} - G' \|_2 \geq \Delta \right) \\
\leq \mathbb{P}\left( W_1(\hat{\epsilon}(\mu_0^m), \rho_a \times \mathcal{N}(0, m_1^{1-2\alpha}G^{m_1})) \geq \frac{1}{2} \epsilon \right| \| G^{m_1} - G' \|_2 < \Delta \) + \mathbb{P}\left( \| G^{m_1} - G' \|_2 \geq \Delta \right) \\
\leq C_1 e^{-C_2 \epsilon^{2}\max(n'+1,4)m_2} + C_3(n')^2 e^{-C_4 \min(\lambda_{\max}(G'), C_5 \lambda_{\max}(G'))^2}m_1.
\end{align*}
\]

Thus, with any pair of increasing \( \mathbb{N}_+ \)-valued sequences \( \{m_{1,k}\}_{k \in \mathbb{N}_+} \) and \( \{m_{2,k}\}_{k \in \mathbb{N}_+} \), denoting \( m_k = (m_{1,k}, m_{2,k}) \), there is

\[
\sum_{k=1}^{\infty} \mathbb{P}\left( W_1(\hat{\epsilon}(\mu_0^{m_k}), \hat{\epsilon}(\mu_0)) > \epsilon \right) < \infty.
\]

Since this holds for any \( \epsilon > 0 \), the Borel-Cantelli lemma implies that

\[
\lim_{k \to \infty} W_1(\hat{\epsilon}(\mu_0^{m_k}), \hat{\epsilon}(\mu_0)) = 0,
\]

almost surely, and hence \( \hat{\epsilon}(\mu_0^{m_k}) \) converges weakly to \( \hat{\epsilon}(\mu_0) \) almost surely.

**B Proof of Lemma 5**

Two parts of Lemma 5 need to be proved: the LLN as \( m_1, m_2 \to \infty \) and the existence of \( \mathcal{G}\mathcal{P}(0, \mathcal{G}) \) as a probability measure on \( \mathcal{C} \).
Part 1: Convergence as $m_1, m_2 \to \infty$

Let $\{x'_1, \ldots, x'_{n'}\}$ be any finite subset of $X$. We write $G' = G[x'_1, \ldots, x'_{n'}]$, $G'^{m_1} = G^{m_1}[x'_1, \ldots, x'_{n'}]$, $e^\Lambda = e_{x'_1, \ldots, x'_{n'}}$ and $\hat{e}^\Lambda = \hat{e}_{x'_1, \ldots, x'_{n'}}$. Let $\lambda_1 \geq \cdots \geq \lambda_{n'}$ be the eigenvalues of $G'$, and $\lambda_1 \geq \cdots \geq \lambda_{n'}$ be the eigenvalues of $G'^{m_1}$. Let $\eta = \min_{k, \in \{0, \ldots, n'\}} |\lambda_k - \lambda_1|$. Recall that when $\alpha = \frac{1}{2}$, $\hat{e}^\Lambda(\mu_0) = \rho_a \times \mathcal{N}(0, G')$. By the triangle inequality of 1-Wasserstein distance, there is

$$W_1(\hat{e}^\Lambda(\mu_0^m), \hat{e}^\Lambda(\mu_0)) = W_1(\hat{e}^\Lambda(\mu_0^m), \rho_a \times \mathcal{N}(0, G')) \leq W_1(\rho_a \times \mathcal{N}(0, G'^{m_1}), \rho_a \times \mathcal{N}(0, G'))$$

$$+ W_1(\hat{e}^\Lambda(\mu_0^m), \rho_a \times \mathcal{N}(0, G'^{m_1})) \leq 2W_1(\mathcal{N}(0, G'^{m_1}), \mathcal{N}(0, G'))$$

First, we examine the first term on the right-hand side. By the property of Wasserstein distances on product measures (e.g. Lemma 3 in [47]), we have

$$W_1(\rho_a \times \mathcal{N}(0, G'^{m_1}), \rho_a \times \mathcal{N}(0, G')) \leq W_1(\rho_a, \rho_a) + W_1(\mathcal{N}(0, G'^{m_1}), \mathcal{N}(0, G'))$$

$$\leq W_1(\mathcal{N}(0, G'^{m_1}), \mathcal{N}(0, G'))$$

Before establishing an upper bound on the 1-Wasserstein distance between $\mathcal{N}(0, G'^{m_1})$ and $\mathcal{N}(0, G')$, we first prove that the $G'^{m_1}$ and $G'$ are close in terms of eigen-decomposition.

**Lemma 23.** If $\|G'^{m_1} - G'\| \leq \frac{1}{2} \eta$, then there exist eigen-decompositions of $G'$ and $G'^{m_1}$, $G' = V \bar{\Lambda} \bar{V}^\top$ and $G'^{m_1} = V \bar{\Lambda} \bar{V}^\top$, where $\bar{V} = [v_1, \ldots, \bar{v}_{n'}] \in \mathbb{R}^{n' \times n'}$ and $\bar{V} = [v_1, \ldots, \bar{v}_{n'}] \in \mathbb{R}^{n' \times n'}$ are both orthonormal matrices, and $\bar{\Lambda}$ and $\Lambda$ are both diagonal matrices, such that $\forall k \in [n'], \bar{v}_k^\top \cdot v_k \geq 1 - \left( \frac{2\|G'^{m_1} - G'\|_2}{\eta} \right)^2$.

**Proof of Lemma 23:** Let $G' = \bar{U} \Sigma \bar{U}^\top$ be any eigen-decomposition of $G'$, where the diagonal entries of $\Sigma$ are sorted in non-ascending order. Account for the possible multiplicity of the eigenvalues, we can write $\Sigma$ as a block-diagonal matrix of the form $\Sigma = \text{diag}(\Sigma_1, \ldots, \Sigma_p)$, where $\forall q \in [p]$, $\Sigma_q$ is a $d_q \times d_q$ diagonal matrix with all diagonal entries equal to some value $\zeta_q$, such that $\zeta_1 > \cdots > \zeta_p > 0$ and moreover, $\sum_{q=1}^p d_q = n'$. We then write $G' = \bar{U} [\bar{U}_1, \ldots, \bar{U}_p]$, where $\forall k \in [p], \bar{U}_q \in \mathbb{R}^{n' \times d_q}$.

Meanwhile, let $G'^{m_1} = U \Sigma U^\top$ be any eigen-decomposition of $G'^{m_1}$, where the diagonal entries are sorted in non-ascending order. Like with $\Sigma$ and $\bar{U}$, we can also write $\Sigma = \text{diag}(\Sigma_1, \ldots, \Sigma_p)$ and $U = [U_1, \ldots, U_p]$, where $\forall q \in [p], \Sigma_q \in \mathbb{R}^{d_q \times d_q}$ and $U_q \in \mathbb{R}^{n' \times d_q}$. Note that unlike in $\Sigma_q$, each $\Sigma_q$ does not necessarily have all its diagonal entries equal.

By the definition of $\eta$, we know that $q, q' \in [p]$ such that $q \neq q'$, there is $|\zeta_q - \zeta_{q'}| \geq \eta$. By Weyl’s inequality for the eigenvalues of perturbed symmetric matrices, we know that $\forall p \in [n'], \|\Sigma_p - \Sigma_p\|_2 \leq \|G'^{m_1} - G'\|_2$. As a result, if $\|G'^{m_1} - G'\|_2 \leq \frac{1}{2} \eta$, then $\forall q, q' \in [p]$ such that $q \neq q'$, we know that $\forall r \in [d_q], \forall r' \in [d_{q'}]$, there is $|\Sigma_q(r) - \Sigma_{q'}(r')| < \frac{1}{2} \eta$. Then, applying the “$\sin(\theta)$ Theorem” of Davis-Kahan [18], we know that $\forall q \in [p]$, the $d_q \times d_q$ matrix $U_q^\top \cdot U_q$ admits a singular value decomposition $E_q \cdot \text{diag}(\cos(\theta_q)) \cdot F_q^\top$, where $E_q, F_q \in \mathbb{R}^{d_q \times d_q}$ are orthonormal matrices and $\theta \in \mathbb{R}^{d_q}$ with each entry in $[0, \frac{\pi}{2}]$, which satisfies

$$\|\sin(\theta_q)\|_\infty \leq \frac{2\|G'^{m_1} - G'\|_2}{\eta},$$

where the $\cos$ and $\sin$ functions are applied entry-wise to the vector $\theta$. Thus, wince the entries of $\theta$ are in $[0, \frac{\pi}{2}]$, we know that $\|1 - \cos(\theta_q)\|_\infty \leq \|1 - \cos^2(\theta_q)\|_\infty \leq \|\sin^2(\theta_q)\|_\infty \leq (\frac{2\|G'^{m_1} - G'\|_2}{\eta})^2$. Defining $\bar{V}_q = \bar{U}_q \cdot E_q$ and $V_q = U_q \cdot F_q$, we then have

$$\bar{V}_q^\top \cdot V_q = E_q^\top \cdot E_q \cdot \text{diag}(\cos(\theta_q)) \cdot F_q^\top \cdot F_q = \text{diag}(\cos(\theta_q)) \cdot F_q^\top \cdot F_q = \text{diag}(\cos(\theta_q)) \cdot F_q^\top \cdot F_q = \text{diag}(\cos(\theta_q)) \cdot F_q^\top \cdot F_q = \text{diag}(\cos(\theta_q)) \cdot F_q^\top \cdot F_q = \text{diag}(\cos(\theta_q)) \cdot F_q^\top \cdot F_q = \text{diag}(\cos(\theta_q)).$$
Thus, writing $\tilde{V} = [\tilde{V}_1, ..., \tilde{V}_p]$ and $V = [V_1, ..., V_p] \in \mathbb{R}^{n' \times n'}, \tilde{\Lambda} = \text{diag}(E_1^\top \cdot \tilde{\Sigma}_1 \cdot E_1, ..., E_p^\top \cdot \tilde{\Sigma}_p \cdot E_p)$ and $\Lambda = \text{diag}(F_1^\top \cdot \Sigma_1 \cdot F_1, ..., F_p^\top \cdot \Sigma_p \cdot F_p)$, we see that

$$G' = \tilde{U} \cdot \tilde{\Sigma} \cdot U^\top = \sum_{q=1}^{p} \tilde{U}_q \cdot \tilde{\Sigma}_q \cdot \tilde{U}_q^\top$$

$$= \sum_{q=1}^{p} (\tilde{U}_q \cdot E_q) \cdot (E_q^\top \cdot \tilde{\Sigma}_q \cdot E_q) \cdot (E_q^\top \cdot \tilde{U}_q^\top)$$

$$= \sum_{q=1}^{p} \tilde{V}_q \cdot (E_q^\top \cdot \tilde{\Sigma}_q \cdot E_q) \cdot \tilde{V}_q = \tilde{V} \cdot \tilde{\Lambda} \cdot \tilde{V}^\top,$$

and similarly, $G'^{m_1} = V \cdot \Lambda \cdot V^\top$, which give eigen-decompositions of $G'$ and $G'^{m_1}$. In particular, $\forall k \in [n']$, if $\tilde{v}_k$ and $v_k$ are the $k$th columns of $\tilde{V}$ and $V$, respectively, then we have $|1 - \tilde{v}_k^\top \cdot v_k| \leq \frac{2\|G'^{m_1} - G'\|_2}{\eta}$. This proves the lemma. $\blacksquare$

With this lemma, we can prove an upper-bound on the 1-Wasserstein distance between $\mathcal{N}(0, G')$ and $\mathcal{N}(0, G'^{m_1})$.

**Lemma 24.** If $\|G'^{m_1} - G'\|_2 < \frac{1}{2\eta}$, then

$$W_1(\mathcal{N}(0, G'^{m_1}), \mathcal{N}(0, G')) \leq \sqrt{n'} \left(\|G'^{m_1} - G'\|_2 + \frac{8\lambda_{\max}\|G'^{m_1} - G'\|_2^2}{\eta^2} + \frac{8\|G'^{m_1} - G'\|_2^2}{\eta^2}\right).$$

**Proof** Using the eigen-decompositions of $G'$ and $G'^{m_1}$ constructed in the proof of Lemma 23, we can apply Lemma 2.4 of [9] to bound the 1-Wasserstein distance between $\mathcal{N}(0, G')$ and $\mathcal{N}(0, G'^{m_1})$:

$$W_1(\mathcal{N}(0, G'^{m_1}), \mathcal{N}(0, G'))$$

$$\leq \sqrt{\sum_{k=1}^{n'} (\sqrt{\lambda_k} - \sqrt{\tilde{\lambda}_k})^2 + 2\sqrt{\lambda_k} \tilde{\lambda}_k (1 - \tilde{v}_k^\top \cdot v_k)}$$

$$\leq \sum_{k=1}^{n'} |\lambda_k - \tilde{\lambda}_k| + 2\max\{\lambda_k, \tilde{\lambda}_k\} (1 - \tilde{v}_k^\top \cdot v_k)$$

$$\leq \sqrt{n'} \left(\|G'^{m_1} - G'\|_2 + 2(\lambda_{\max} + \|G'^{m_1} - G'\|_2)\frac{2\|G'^{m_1} - G'\|_2}{\eta}\right)^2$$

$\blacksquare$

Next, we look at the second term on the right-hand side of \[(38)\]. We see that, when conditioned on $z_1, ..., z_{m_2}$, \(\{[a_0^i, h_0^i(x_{i1}^i), ..., h_0^i(x_{i_k}^i)]\}_{i \in [m_2]}\) is distributed i.i.d. across $i \in [m_2]$ according to $\rho_0 \times \mathcal{N}(0, G'^{m_1})$. Hence, conditioned on $G'^{m_1}$, which is measurable with respect to $z_1, ..., z_{m_2}$, $\hat{e}^k(\mu^m_0)$ has the same distribution as the empirical measure of $m_2$ i.i.d. samples from $\rho_0 \times \mathcal{N}(0, G'^{m_1})$, which we denote by $\nu^m_{(m_2)} \in \mathcal{P}(\mathbb{R} \times \mathbb{R}^{n'})$. Therefore, by conditioning on $G'^{m_1}$, we can again leverage concentration inequalities of empirical measures of i.i.d. samples in Wasserstein distance, as given by Lemma 22. In particular, we choose $d = n' + 1, \nu = \rho_0 \times \mathcal{N}(0, G'^{m_1})$ and choose $\alpha = 2,$
\[ \gamma = \frac{1}{\lambda_{\max}(G_{m1})}. \]

Recalling that \( \mathcal{N}(0, G_{m1}) \) is also the distribution \( (G_{m1})^{\frac{1}{2}} \cdot u \), where each entry of \( u \in \mathbb{R}^n \) is independently distributed as \( \mathcal{N}(0, 1) \), we can then write

\[
\mathcal{E}_{\alpha, \gamma}(\nu) = \int_{\mathbb{R}} \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{\gamma(a^2 + \|G_{m1}\|^{\frac{1}{2}} \cdot u)^{\frac{1}{2}}} e^{-\|u\|_2^2} \, du \, \rho_u(da)
\]

\[
\leq e^{\gamma(a_{max}^0)^2} \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{(\gamma \lambda_{\max}(G_{m1}) - 1)\|u\|_2^2} \, du
\]

\[
\leq e^{\gamma(a_{max}^0)^2} \frac{2^\nu}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-\|u\|_2^2/2} \, du
\]

\[
\leq 2^\nu e^{\gamma(a_{max}^0)^2/(2\lambda_{\max}(G_{m1}))} < \infty.
\]

Moreover, for \( u > 0 \), \( \log(2 + \frac{1}{u}) < 1 + \frac{1}{u} \), and hence \( \frac{u}{\log(2 + \frac{1}{u})} \geq \frac{u^2}{u+1} \geq u^2 \). Therefore, applying Lemma 22, we have \( \forall u > 0, \exists C_1, C_2 > 0 \) such that

\[
P\left(\mathcal{W}_1(\hat{e}(\mu_0^m), \rho_u \times \mathcal{N}(0, G_{m1})) \geq u \mid G_{m1}\right) = P\left(\mathcal{W}_1(\mathcal{V}(m_2), \nu) \geq u \mid G_{m1}\right)
\]

\[
\leq C_1 e^{-C_2 m_2 \mu_{\max}(n'+1, 4)}
\]

where \( C_1 \) and \( C_2 \) depend on \( n', a_{max}^0 \) and \( \lambda_{\max}(G_{m1}) \).

Furthermore, if we condition on the event that \( \|G_{m1} - G'\|_2 < \Delta \) for any \( \Delta \in (0, \lambda_{\max}(G')) \) – which is measurable with respect to \( G_{m1} \) – then by choosing \( \alpha = 2 \) and \( \gamma = \frac{1}{\lambda_{\max}(G')} \), we have \( \mathcal{E}_{\alpha, \gamma}(\nu) \leq 2^\nu e^{\gamma(a_{max}^0)^2/(2\lambda_{\max}(G_{m1}))} < \infty \). Therefore, \( \forall u > 0, \exists C_1, C_2 > 0 \) depending only on \( n', a_{max}^0 \) and \( \lambda_{\max}(G') \) such that

\[
P\left(\mathcal{W}_1(\hat{e}(\mu_0^m), \rho_u \times \mathcal{N}(0, G_{m1})) \geq u \left\|G_{m1} - G'\right\|_2 < \Delta \right) \leq C_1 e^{-C_2 m_2 \mu_{\max}(n'+1, 4)}.
\]

Thus, our overall strategy is to control the first and second terms on the right-hand side of (38) via Lemma 24 and (39), respectively, by restricting to the high-probability event that \( \|G_{m1} - G'\|_2 < \Delta \) for some \( \Delta > 0 \). Specifically, we will use the following concentration result of \( G_{m1} \):

**Lemma 25** ([11], Lemma 4). Let \( \{x_1', \ldots, x_{n'}\} \) be any finite subset of \( \mathcal{X} \). Let \( G' = \mathcal{G}[x_1', \ldots, x_{n'}] \) and \( G_{m1} = \mathcal{G}[x_1', \ldots, x_{n'}] \). \( \exists C_3, C_4, C_5 > 0 \), which depend on \( L_o \) and the sub-Gaussian norm of \( \rho_u \) such that, \( \forall \Delta > 0 \)

\[
P\left( \left\|G_{m1} - G'\right\|_2 \geq \Delta \right) < C_3(n')^2 e^{-C_4 \min(\Delta, C_5 \Delta^2)m_1}.
\]

Fix an \( \epsilon > 0 \). Define

\[
\Delta_\epsilon = \min \left\{ \frac{1}{2} \eta, \frac{e^2(\lambda_{\min}(G'))^{\frac{1}{2}}}{12n'}, \frac{\epsilon \eta}{(96n'\lambda_{\max}(G'))^{\frac{1}{2}}}, \left( \frac{e^2 \eta^2}{96n'} \right)^{\frac{1}{2}}, \left( \frac{e^2 \eta^2}{96n'} \right)^{\frac{1}{2}} \right\}
\]

Then, conditioned on the event that \( \|G_{m1} - G'\|_2 \leq \Delta \), it holds that \( \|G_{m1} - G'\|_2 \leq \frac{1}{2} \eta \) and \( \mathcal{W}_1(\mathcal{N}(0, G_{m1}), \mathcal{N}(0, G')) \leq \frac{1}{2} \epsilon \). Thus, putting things together,

\[
P\left( \mathcal{W}_1(\hat{e}(\mu_0^m), \hat{e}(\mu_0)) > \epsilon \right)
\]

\[
\leq P\left( \mathcal{W}_1(\hat{e}(\mu_0^m), \hat{e}(\mu_0)) > \epsilon \mid \|G_{m1} - G'\|_2 < \Delta_\epsilon \right) + P\left( \|G_{m1} - G'\|_2 \geq \Delta_\epsilon \right)
\]

\[
\leq P\left( \mathcal{W}_1(\hat{e}(\mu_0^m), \rho_u \times \mathcal{N}(0, G_{m1})) \geq \frac{1}{2} \epsilon \mid \|G_{m1} - G'\|_2 < \Delta_\epsilon \right) + P\left( \|G_{m1} - G'\|_2 \geq \Delta_\epsilon \right)
\]

\[
\leq C_1 e^{-C_2 (\epsilon/2)^{\max(n'+1, 4)}m_2} + C_3(n')^2 e^{-C_4 \min(\Delta, C_5 \Delta^2)m_1}.
\]
Thus, with any pair of increasing \( N_+ \)-valued sequences \( \{ m_{1,k} \}_{k \in \mathbb{N}_+} \) and \( \{ m_{2,k} \}_{k \in \mathbb{N}_+} \), denoting \( m_k = (m_{1,k}, m_{2,k}) \), there is
\[
\sum_{k=1}^{\infty} \mathbb{P} \left( W_1(\hat{e}(\mu_0^{m_k}), \hat{e}(\mu_0)) > \epsilon \right) < \infty .
\]
Since this holds for any \( \epsilon > 0 \), the Borel-Cantelli lemma implies that
\[
\lim_{k \to \infty} W_1(\hat{e}(\mu_0^{m_k}), \hat{e}(\mu_0)) = 0 ,
\]
amost surely, and hence \( \hat{e}(\mu_0^{m_k}) \) converges weakly to \( \hat{e}(\mu_0) \) almost surely.

**Part 2: Existence of \( \mathcal{GP}(0, \mathcal{G}) \) as a probability measure on \( \mathcal{C} \)**

Since the set of all given finite-dimensional distributions clearly satisfy the consistency conditions for a projective family of probability measures, the Kolmogorov extension theorem (e.g. Theorem 5.16 in [39]) implies that there exists a random field with \( \mathcal{X} \) being the index space, \( \{ \mathcal{B}_x \}_{x \in \mathcal{X}} \), such that \( \forall x_1, \ldots, x_{\ell'}, \) the random vector \( \{ \mathcal{B}_{x_1}, \ldots, \mathcal{B}_{x_{\ell'}} \} \) is distributed as \( \mathcal{N}(0, \mathcal{G}[x_1, \ldots, x_{\ell'}]) \).

It remains to apply the Kolmogorov-Chentsov continuity theorem (e.g. Theorem 2.23 in [39]) to prove that there exists a continuous version of \( B \). Note that \( \forall x_1, x_2 \in \mathcal{X}, \mathcal{B}_{x_1} - \mathcal{B}_{x_2} \) follows a Gaussian distribution with mean zero and variance
\[
\text{Var}(\mathcal{B}_{x_1} - \mathcal{B}_{x_2}) = \mathcal{G}(x_1, x_1) + \mathcal{G}(x_2, x_2) - \mathcal{G}(x_2, x_2)
\]
\[
= \mathbb{E}_{z \in \rho_x} [\sigma(z^\top x_1)\sigma(z^\top x_2) + \sigma(z^\top x_2)\sigma(z^\top x_2) - 2\sigma(z^\top x_1)\sigma(z^\top x_2)]
\]
\[
= \mathbb{E}_{z \in \rho_x} [(\sigma(z^\top x_1) - \sigma(z^\top x_2))^2]
\]
\[
\leq \mathbb{E}_{z \in \rho_x} [(z^\top (x_1 - x_2))^2]
\]
\[
\leq \mathbb{E}_{z \in \rho_x} \|z\|_{\mathcal{S}}^2 \|x_1 - x_2\|^2 ,
\]
where \( \|\rho_x\|_{\mathcal{S}} < \infty \) is the sub-Gaussian norm of \( \rho_x \) [72]. Thus, \( \forall p \in \mathbb{N}_+ \),
\[
\mathbb{E} \left[ |\mathcal{B}_{x_1} - \mathcal{B}_{x_2}|^{2p} \right] \leq (p-1)!! (\text{Var}(\mathcal{B}_{x_1} - \mathcal{B}_{x_2}))^p C_p \|x_1 - x_2\|^{2p} ,
\]
with some constant \( C_p > 0 \). Therefore, by the Kolmogorov-Chentsov continuity theorem, there exists a version of \( B \) whose sample paths are locally Hölder continuous with exponent \( \frac{2p-d}{2p} \). In fact, since this argument applies to all \( p \in \mathbb{N}_+ \), we know that \( \forall \alpha \in [0, 1) \), there exists a version of \( B \) whose sample paths are locally Hölder continuous with exponent \( \alpha \). In particular, there exists a version of \( B \) whose sample paths are continuous, since Hölder continuity with any exponent \( \alpha > 0 \) implies uniform continuity. Then, the law of sample paths of such a \( B \) is indeed supported on \( \mathcal{C} \).

**C Proof of Lemma 6**

The dynamics of \( \nu_t \) is a Wasserstein gradient flow on finite-dimensional Euclidean space, whose existence has been proved in prior works such as [7, 50, 70]. Below, we prove that the characteristic flow maps \( A_t \) and \( H_t \) constructed from \( \nu_t \) via (18) and (21) indeed satisfy (9) and (10).

First, as an intermediate step, we construct a candidate for \( \hat{e}_\Delta \# \mu_\Delta \) from \( \nu_\Delta \). For \( t \geq 0 \), we define two maps, \( A_t^\Delta : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R} \) and \( U_t^\Delta = [U_{t,1}^\Delta, \ldots, U_{t,n}^\Delta] : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n \), by
\[
A_t^\Delta (a, u) = C_t(a, (G^+)^{\frac{1}{2}} \cdot u) , \tag{40}
\]
\[
U_t^\Delta (a, u) = G^{\frac{1}{2}} \cdot \Lambda_t(a, (G^+)^{\frac{1}{2}} \cdot u) , \tag{41}
\]
for \((a, u) \in \text{supp}(\mu_{0, \triangle})\). We let \(\Theta^\triangle_t = [A^\triangle_t, U^\triangle_t] : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R} \times \mathbb{R}^n\), and want to show that
\[
A^\triangle_t(a, u) = a, \quad U^\triangle_0(a, u) = u, \quad \quad (42)
\]
\[\frac{d}{dt} A^\triangle_t(a, u) = -\frac{1}{n} \sum_{k=1}^n \sigma(U^\triangle_{t,k}(a, u))(f^\triangle_{t,k} - y_k), \quad \quad (43)\]
\[\frac{d}{dt} U^\triangle_{t,k}(a, u) = -\frac{1}{n} A^\triangle_t(a, u) \sum_{k=1}^n \sigma'(U^\triangle_{t,k}(a, u))(f^\triangle_{t,k} - y_k)\ G_{kl}, \quad \quad (44)\]

if we define \(\mu_{t, \triangle} = (\Theta^\triangle_t)\#\mu_{0, \triangle}\) and \(f^\triangle_{t,k} = \int_{\mathbb{R} \times \mathbb{R}^n} a \sigma(u_k) \mu_{t, \triangle}(da, du)\). First, there is
\[
f^\triangle_{t,k} = \int_{\mathbb{R} \times \mathbb{R}^n} A^\triangle_t(a, u) \sigma'(U^\triangle_{t,k}(a, u)) \mu_{0, \triangle}(da, du) \]
\[= \int_{\mathbb{R} \times \mathbb{R}^n} C_t(a, (G^+)^{\frac{1}{2}} \cdot u) \sigma'((G^+)^{\frac{1}{2}} \cdot \Lambda_t(a, (G^+)^{\frac{1}{2}} \cdot u)) \mu_{0, \triangle}(da, du) \]
\[= \int_{\mathbb{R} \times \mathbb{R}^n} C_t(a, \lambda) \sigma'(\Lambda_t(a, \lambda)^\top \cdot \bar{x}_k) \nu_0(da, d\lambda) \]
\[= \int_{\mathbb{R} \times \mathbb{R}^n} a \sigma'((\lambda^\top \cdot \bar{x}_k)) \nu_t(da, d\lambda) = g_t(\bar{x}_k) .\]

Recall that \(\mu_{0, \triangle} = \rho_a \times N(0, G)\) if \(\alpha = \frac{1}{2}\) and \(\rho_a \times \delta_0\) if \(\alpha > \frac{1}{2}\). Hence, in either case, if \((a, u) \in \text{supp}(\mu_{0, \triangle})\), then \(u\) belongs to the range of \(G^\frac{1}{2}\), which implies that \(G^\frac{1}{2} \cdot (G^+)^{\frac{1}{2}} \cdot u = u\). Thus, for any \((a, u) \in \text{supp}(\mu_{0, \triangle})\), there is \(A^\triangle_0(a, u) = C_0(a, (G^+)^{\frac{1}{2}} \cdot u) = a\) and \(U^\triangle_0(a, u) = G^\frac{1}{2} \cdot \Lambda_0(a, (G^+)^{\frac{1}{2}} \cdot u) = G^\frac{1}{2} \cdot (G^+)^{\frac{1}{2}} \cdot u = u\). Moreover, it holds that
\[
\frac{d}{dt} A^\triangle_t(a, u) = \frac{d}{dt} C_t(a, (G^+)^{\frac{1}{2}} \cdot u) \]
\[= -\frac{1}{n} \sum_{k=1}^n (g_t(\bar{x}_k) - y_k) \sigma(\Lambda_t(a, (G^+)^{\frac{1}{2}} \cdot u)^\top \cdot \bar{x}_k) \]
\[= -\frac{1}{n} \sum_{k=1}^n (f^\triangle_{t,k} - y_k) \sigma(U^\triangle_{t,k}(a, u)), \]

and
\[
\frac{d}{dt} U^\triangle_{t,k}(a, u) = \left( G^\frac{1}{2} \cdot \frac{d}{dt} \Lambda_t(a, (G^+)^{\frac{1}{2}} \cdot u) \right)_l \]
\[= -\frac{1}{n} \sum_{k=1}^n (g_t(\bar{x}_k) - y_k) \sigma'(\Lambda_t(a, (G^+)^{\frac{1}{2}} \cdot u)^\top \cdot \bar{x}_k) (G^\frac{1}{2} \cdot \bar{x}_k)_l \]
\[= -\frac{1}{n} A^\triangle_t(a, u) \sum_{k=1}^n (f^\triangle_{t,k} - y_k) \sigma'(U^\triangle_{t,k}(a, u)) G_{kl} , \]

which verify (43) and (44). In addition,
\[
\frac{d}{dt} U^\triangle_t(a, u) = -\frac{1}{n} A^\triangle_t(a, u) G \cdot \left( (f^\triangle_{t,k} - y_k) \sigma'(U^\triangle_{t,k}) \right)_{k=1}^n , \]

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and hence
\[
U_t^\Delta(a, u) = u - G \cdot \frac{1}{n} \int_0^t A^\Delta_s(a, u) \left[ (f_{s,k} - y_k) \sigma'(U^\Delta_{s,k}(a, u)) \right]_{k=1}^n ds
\]
belongs to the range of \( G \) for all \( t \geq 0 \). We also observe from (40) and (41) that for \((a, u) \in \mu_{0, \Delta}, (G^+)^{\frac{1}{2}}(\Theta_t^\Delta(a, u)) = \Lambda_t((G^+)^{\frac{1}{2}}(a, u))\), and therefore,
\[
\nu_t = (A_t)_#((G^+)^{\frac{1}{2}})_\#\mu_{0, \Delta} = ((G^+)^{\frac{1}{2}})_#(\Theta_t^\Delta)_#\mu_{0, \Delta} = ((G^+)^{\frac{1}{2}})_#\mu_{t, \Delta}.
\]
Next, we will construct \( \mu_t \) from \( \mu_{t, \Delta} \), by defining, for \((a, h) \in \text{supp}(\mu_0)\),
\[
A_t(a, h) = A_t^\Delta(a, e(h)) = C_t(a, (G^+)^{\frac{1}{2}} \cdot e(h)), \tag{45}
\]
and
\[
H_t(a, h) = h + \sum_{k=1}^n \left( G^+ \cdot \left( U_t^\Delta(a, e(h)) - e(h) \right) \right)_k G(x_k, \cdot)
\]
\[
= h + \sum_{k=1}^n \left( (G^+)^{\frac{1}{2}} \cdot \left( A_t(a, (G^+)^{\frac{1}{2}} \cdot e(h)) - (G^+)^{\frac{1}{2}} \cdot e(h)) \right) \right)_k G(x_k, \cdot).
\]
We first check that,
\[
A_0(a, h) = A_0^\Delta(a, e(h)) = a
\]
\[
H_0(a, h) = h + \sum_{k=1}^n \left( G^+ \cdot \left( U_0^\Delta(a, e(h)) - e(h) \right) \right)_k G(x_k, \cdot) = h.
\]
Next, for all \((a, h) \in \text{supp}(\mu_0), e(h) \in \text{range}(G)\), and thus (C) implies that \( U_t^\Delta(a, e(h)) \)
belongs to the range of \( G \) as well. Therefore, \( \forall k \in [n], t \geq 0, \)
\[
H_t(a, h)(x_k) = h(x_k) + \left( G \cdot G^+ \cdot \left( U_t^\Delta(a, e(h)) - e(h) \right) \right)_k
\]
\[
= U_{t,k}^\Delta(a, e(h)), \tag{46}
\]
Moreover,
\[
f_t(x_k) = \int_{R \times C} A_t(a, h) \sigma(H_t(a, h)(x_k)) \mu_0(da, dh)
\]
\[
= \int_{R \times C} A_t^\Delta(a, e(h)) \sigma'(U_{t,k}^\Delta(a, e(h))) \mu_0(da, dh)
\]
\[
= \int_{R \times R^n} A_t^\Delta(a, u) \sigma(U_{t,k}^\Delta(a, u)) \mu_{0, \Delta}(da, du) = f_{t,k}^\Delta,
\]
and hence,
\[
\frac{d}{dt} A_t(a, h) = \frac{d}{dt} A_t^\Delta(a, e(h)) = -\frac{1}{n} \sum_{k=1}^n \left( f_{t,k}^\Delta - y_k \right) \sigma(U_{t,k}^\Delta(a, e(h)))
\]
\[
= -\frac{1}{n} \sum_{k=1}^n \left( f_t(x_k) - y_k \right) \sigma(H_t(a, h)(x_k)).
\]
and
\[
\frac{d}{dt} H_t(a, h) = \sum_{k=1}^{n} \mathcal{G}(x_k, \cdot) \left( G^+ \cdot \frac{d}{dt} U_t^\triangle(a, e(\triangle h)) \right)_k
\]
\[= - \sum_{k=1}^{n} \mathcal{G}(x_k, \cdot) \left( -\frac{1}{n} A^\triangle_t(a, e(\triangle h)) G^+ \cdot G \cdot \left( (f_{t,k} - y_k) \sigma'(U_{t,k}^\triangle(a, e(\triangle h))) \right)_{t=1}^{\infty} \right)_k
\]
\[= - \frac{1}{n} A^\triangle_t(a, e(\triangle h)) \sum_{k=1}^{n} (f_{t,k} - y_k) \sigma'(U_{t,k}^\triangle(a, e(\triangle h))) \mathcal{G}(x_k, \cdot)
\]
\[= - \frac{1}{n} A_t(a, h) \sum_{k=1}^{n} (f_t(x_k) - y_k) \sigma'(H_t(a, h)(x_k)) \mathcal{G}(x_k, \cdot),
\]
which verify (9) and (10). This proves the existence of \( \mu_t \).

Furthermore, (45) and (46) imply that for \((a, h) \in \text{supp}(\mu_0)\), there is
\[
\hat{e}_\triangle(\Theta_t(a, h)) = \Theta^\triangle_t(e(\triangle a, h)).
\]

This implies that, \( \forall t \geq 0, \mu_{t, \triangle} = (\Theta^\triangle_t)_{\#}(e(\triangle))_{\#} \mu_0 = (e(\triangle))_{\#}(\Theta_t)_{\#} \mu_0 = (e(\triangle))_{\#} \mu_t \), and hence also \( \nu_t = ((G^+)^{\frac{1}{2}})_{\#} \mu_{t, \triangle} = ((G^+)^{\frac{1}{2}})_{\#}(e(\triangle))_{\#} \mu_t \). Therefore,
\[
f_t(x) = \int_{\mathbb{R} \times C} A_t(a, h) \sigma(H_t(a, h)(x)) \mu_0(da, dh)
\]
\[= \int_{\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}} A^\triangle_t(a, u) \sigma \left( v + \sum_{k=1}^{n} \left( (G^+)^{\frac{1}{2}} \cdot (A_t(a, (G^+)^{\frac{1}{2}}) \cdot u) - (G^+)^{\frac{1}{2}} \cdot u \right) \right) G(x_k, \cdot) \mu_0(da, du, dv)
\]
\[= \int_{\mathbb{R} \times \mathbb{R}^n} A^\triangle_t(a, u) \mathbb{E}_{Z \sim \mathcal{N}(0, 1)} \left[ \sigma \left( \tau_x Z + \sum_{k=1}^{n} \left( (G^+)^{\frac{1}{2}} \cdot A_t(a, (G^+)^{\frac{1}{2}}) \cdot u \right) \right)_k \mathcal{G}(x_k, \cdot) \right] \mu_0(da, du)
\]
\[= \int_{\mathbb{R} \times \mathbb{R}^n} C_t(a, u) \mathbb{E}_{Z \sim \mathcal{N}(0, 1)} \left[ \sigma \left( \tau_x Z + \sum_{k=1}^{n} \left( (G^+)^{\frac{1}{2}} \cdot A_t(a, \lambda) \right)_k \mathcal{G}(x_k, \cdot) \right] \nu_0(da, d\lambda)
\]
\[= \int_{\mathbb{R} \times \mathbb{R}^n} a \mathbb{E}_{Z \sim \mathcal{N}(0, 1)} \left[ \sigma \left( \tau_x Z + \lambda^T \cdot \hat{X}(x) \right) \right] \nu_t(da, d\lambda).
\]

D Proof of Lemma 8

We define \( \mu_{t, \triangle}^m = (e(\triangle))_{\#} \mu_t^m \). The goal then is to provide an upper bound for \( \mathcal{W}_1(\mu_{t, \triangle}, \mu_{t, \triangle}^m) \). Since \( \mu_t^m \) is obtained via the push-forward of \( \Theta_t^m \), which satisfies (7) and (8), we see that \( \mu_{t, \triangle}^m \) can be written as \( \mu_{t, \triangle}^m = (\Theta_t^{m, \triangle})_{\#} \mu_0^m \), where \( \Theta_t^{m, \triangle} = [A_t^{m, \triangle}, U_t^{m, \triangle}] : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R} \times \mathbb{R}^n \) evolve according to
\[
\frac{d}{dt} A_t^{m, \triangle}(a, u) = -\frac{1}{n} \sum_{k=1}^{n} \sigma(U_{t,k}^{m, \triangle}(a, u)) (f_{t,k} - y_k),
\]
\[
\frac{d}{dt} U_{t,k}^{m, \triangle}(a, u) = -\frac{1}{n} A_t^{m, \triangle}(a, u) \sum_{k=1}^{n} \sigma(U_{t,k}^{m, \triangle}(a, u)) (f_{t,k} - y_k) G_{kl},
\]
\[
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\]
with \(A^\triangle_m(a,u) = a\) and \(U^\triangle_m(a,u) = u_k\), and where \(f^\triangle_{t,k} = \int_{\mathbb{R}^n} a\sigma(u_k)\mu^m_{t,\triangle}(da,du)\). Thus, our strategy is to use the triangle inequality of 1-Wasserstein distance to write

\[
W_1(\mu_{t,\triangle}; \mu^m_{t,\triangle}) = W_1((\Theta_t^\triangle)_\#\mu^m_{t,\triangle} - (\Theta^\triangle_t)_\#\mu^m_{0,\triangle}) \\
≤ W_1((\Theta_t^\triangle)_\#\mu^m_{0,\triangle}) + W_1((\Theta^\triangle_t)_\#\mu^m_{0,\triangle}) \\
= W_1(\mu_{t,\triangle}; \tilde{\mu}^m_{t,\triangle}) + W_1(\mu_{t,\triangle}; \tilde{\mu}^m_{t,\triangle}),
\]

where we define \(\tilde{\mu}^m_{t,\triangle} = (\Theta^\triangle_t)_\#\mu^m_{0,\triangle}\).

To bound the first term on the right-hand side of (50), we use the following inequality:

\[
W_1(\mu_{t,\triangle}; \tilde{\mu}^m_{t,\triangle}) \leq W_1((\Theta^\triangle_t)_\#\mu^m_{0,\triangle}) \leq \text{Lip}(\Theta_t^\triangle) W_1(\mu^m_{0,\triangle}, \mu^m_{0,\triangle}).
\]

To bound \(\text{Lip}(\Theta_t^\triangle)\), we need the following lemma:

**Lemma 26.** For \(n \in \mathbb{N}_+\) and \(t \geq 0\), there exists \(C_1(n,t)\) and \(C_2(n,t)\) that are non-negative and non-decreasing in \(t\) such that \(\forall t \geq 0, \forall a \in \text{supp}(\mu_0), u \in \mathbb{R}^n\),

\[
|A_t^\triangle(a,u)| \leq C_1(n,t), \quad |A^m_t(a,u)| \leq C_1(n,t)
\]

and for all \(x \in \mathcal{X}\),

\[
\sup_{k \in [n]} |f_t(x_k)| \leq C_2(n,t), \quad \sup_{k \in [n]} |f^m_t(x_k)| \leq C_2(n,t)
\]

**Proof** There is

\[
|f^\triangle_{t,k}| \leq M_\sigma \int_{\mathbb{R}^n} |A_t^\triangle(a,u)| \mu_{t,\triangle}(da,du) \\
\leq M_\sigma \sup_{a \in \text{supp}(\mu_0), u \in \mathbb{R}^n} |A_t^\triangle(a,u)|.
\]

Then,

\[
|A_t^\triangle(a,u)| \leq |a| + \int_0^t \frac{1}{n} \sum_{k=1}^n M_\sigma |f^\triangle_{s,k}| \, ds \\
\leq |a| + (M_\sigma)^2 \sup_{a \in \text{supp}(\mu_0), u \in \mathbb{R}^n} |A_s^\triangle(a,u)| \, ds.
\]

Thus, by Grönwall’s inequality, there exists \(C_1(n,t)\) such that

\[
\sup_{a \in \text{supp}(\mu_0), u \in \mathbb{R}^n} |A_t^\triangle(a,u)| \leq C_1(n,t),
\]

and hence \(\forall x \in \mathcal{X}, |f_t(x)| \leq M_\sigma C_1(n,t) = C_2(n,t)\).

Similar arguments apply to \(\sup_{a \in \text{supp}(\mu_0), u \in \mathbb{R}^n} |A^m_t(a,u)|\) and \(f^m_t(x)\).

Define the following ODE for \(z(t) = [z_0(t), \ldots, z_n(t)]^\top \in \mathbb{R}^{n+1}\):

\[
\frac{d}{dt} z(t) = F(z(t)),
\]

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where \( \forall l \in \{0, \ldots, n\} \),

\[
(F(z))_k = \begin{cases} 
- \sum_{l=1}^{n} \sigma(z_l)(f_{t,k} - y_k), & k = 0 \\
- z_0 \sum_{l=1}^{n} \sigma(z_l)(f_{t,k} - y_k) G_{k,l}, & k \in [n].
\end{cases}
\]

Then, \( \Theta^\Delta_t : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R} \times \mathbb{R}^n \) can be considered as the map from the initial condition \( z(0) \) to the solution \( z(t) \) at time \( t \) of this ODE. Recall that the solutions of an ODE with a Lipschitz-continuous function on the right-hand side depends continuously on the initial condition. Since within the interval \( [0, t] \), the function \( F \) is Lipschitz-continuous with Lipschitz constant

\[
\operatorname{Lip}(F) \leq n M_{\sigma}(C_2(n, t) + \|y\|_\infty)(1 + n C_1(n, t)L_{\sigma}M_{\sigma}) =: C_3'(n, t) < \infty,
\]

we know that

\[
\operatorname{Lip}(\Theta^\Delta_t) \leq e^{tC_3'(n, t)} =: C_3(n, t) < \infty.
\]

Thus,

\[
W_1(\mu_{t, \Delta}, \tilde{\mu}_{t, \Delta}) \leq C_3(n, t) W_1(\mu_{0, \Delta}, \mu_{0, \Delta}^m).
\]

Next, we consider the second term on the right-hand side of (50). Define

\[
\Delta A_{t}^{m, \Delta} = \int_{\mathbb{R} \times \mathbb{R}^n} |A_{t}^{m, \Delta}(a, u) - A_{t}^{\Delta}(a, u)|\mu_{0, \Delta}^m(da, du),
\]

\[
\Delta U_{t}^{m, \Delta} = \int_{\mathbb{R} \times \mathbb{R}^n} \|U_{t}^{m, \Delta}(a, u) - U_{t}^{\Delta}(a, u)\|\mu_{0, \Delta}^m(da, du).
\]

Note that at initialization, there is \( \Delta A_{0}^{m, \Delta} = \Delta U_{0}^{m, \Delta} = 0 \). For the second term on the right-hand side of (50), we then see that

\[
W_1(\mu_{t, \Delta}, \tilde{\mu}_{t, \Delta}) \leq \left( \int_{\mathbb{R} \times \mathbb{R}^n} \|\Theta_{t}^{m, \Delta}(a, u) - \Theta_{t}^{\Delta}(a, u)\|\mu_{0, \Delta}^m(da, du) \right)^{1/2} \]

\[
\leq \Delta A_{t}^{m, \Delta} + \Delta U_{t}^{m, \Delta}.
\]

Therefore, from (50), we deduce that that

\[
W_1(\mu_{t, \Delta}, \tilde{\mu}_{t, \Delta}) \leq C_3(n, t) W_1(\mu_{0, \Delta}, \mu_{0, \Delta}^m) + \Delta A_{t}^{m, \Delta} + \Delta U_{t}^{m, \Delta}.
\]

Moreover, (48) and (43) imply that

\[
\frac{d}{dt} |A_{t}^{m, \Delta}(a, u) - A_{t}^{\Delta}(a, u)|
\]

\[
\leq \sum_{k=1}^{n} |\sigma((U_{t}^{m, \Delta}(a, u))) - \sigma((U_{t}^{\Delta}(a, u)))| \left( \sup_{k \in [n]} |f_t(x_k)| + \|y\|_\infty \right)
\]

\[
+ \sum_{k=1}^{n} |\sigma((U_{t}^{m, \Delta}(a, u)))| \sup_{k \in [n]} |f_t^{m}(x_k) - f_t(x_k)|
\]

\[
\leq L_{\sigma}(C_2(n, t) + \|y\|_\infty) \Delta U_{t}^{m, \Delta} + n M_{\sigma} L_{\sigma} C_1(n, t) + M_{\sigma} W_1(\mu_{t, \Delta}, \tilde{\mu}_{t, \Delta})
\]

\[
\leq n M_{\sigma} L_{\sigma} C_1(n, t) |A_{t}^{m, \Delta}(a, u) - A_{t}^{\Delta}(a, u)| + n(M_{\sigma})^2 \Delta A_{t}^{m, \Delta}
\]

\[
+ (L_{\sigma}(C_2(n, t) + \|y\|_\infty) + n M_{\sigma} L_{\sigma} C_1(n, t) + M_{\sigma}) \Delta U_{t}^{m, \Delta}
\]

\[
+ n M_{\sigma}(L_{\sigma} C_1(n, t) + M_{\sigma}) C_3(n, t) W_1(\mu_{0, \Delta}^m, \mu_{0, \Delta}).
\]
Meanwhile, (49) and (44) imply that, \(\forall k \in [n]\),
\[
\left| \frac{d}{dt} \left( U_{t,l}^{m,\Delta}(a, u) - U_{l,l}^{\Delta}(a, u) \right) \right| \\
\leq \left| A_t^{m,\Delta}(a, u) - A_t^{\Delta}(a, u) \right| \sum_{k=1}^{n} \left| \sigma'(U_{t,k}^{\Delta}(a, u)) \right| \left| f_{t,k}^{\Delta} - y_k \right| |G_{kl}| \\
+ \left| A_t^{m,\Delta}(a, u) \right| \sum_{k=1}^{n} \left| \sigma'(U_{t,k}^{\Delta}(a, u)) - \sigma'(U_{t,k}^{m,\Delta}(a, u)) \right| \left| f_{t,k}^{\Delta} - y_k \right| |G_{kl}| \\
+ \left| A_t^{m,\Delta}(a, u) \right| \sum_{k=1}^{n} \left| \sigma'(U_{t,k}^{m,\Delta}(a, u)) \right| \left| (f_{t,k}^{\Delta} - y_k) - (f_{t,k}^{m,\Delta} - y_k) \right| |G_{kl} - G_{kl}^{m,\Delta}| \\
\leq nL_{\sigma}(\sigma)^2(C_2(n,t) + \|y\|_\infty)\Delta A_t^{m,\Delta} \\
+ L_{\sigma}(\sigma)^2C_1(n,t)(C_2(n,t) + \|y\|_\infty)\Delta U_t^{m,\Delta} \\
+ nL_{\sigma}(\sigma)^2C_1(n,t)(M_\sigma + C_1(n,t)L_\sigma)(C_3(n,t) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m,\Delta}) + \Delta A_t^{m,\Delta} + \Delta U_t^{m,\Delta}) \\
+ \sqrt{nL_{\sigma}}C_1(n,t)(C_2(n,t) + \|y\|_\infty)\|G - G^{m,\Delta}\|_2.
\]

where we use the inequality that \(\forall k \in [n]\),
\[
\left| f_{t,k}^{m,\Delta} - f_{t,k}^{\Delta} \right| = \int_{\mathbb{R} \times \mathbb{R}^n} a\sigma(u_k)(\mu_{t,\Delta}^{m,\Delta} - \mu_{t,\Delta})(da, du) \\
\leq (\sigma + C_1(n,t)L_\sigma) W_1(\mu_{0,\Delta}, \mu_{t,\Delta}) \\
\leq (\sigma + C_1(n,t)L_\sigma)(C_3(n,t) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m,\Delta}) + \Delta A_t^{m,\Delta} + \Delta U_t^{m,\Delta}).
\]

Together, (51) and (52) imply that
\[
\Delta A_t^{m,\Delta} + \Delta U_t^{m,\Delta} \\
\leq \int_0^t \left( C_4(n,s)(\Delta A_s^{m,\Delta} + \Delta U_s^{m,\Delta}) + C_5(n,s) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m,\Delta}) + C_6(n,t)\|G^{m,\Delta} - G\|_2 \right) ds.
\]

Thus, by Grönwall’s inequality, we have
\[
\Delta A_t^{m,\Delta} + \Delta U_t^{m,\Delta} \leq C_5(n,t) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m,\Delta}) + C_6(n,t)\|G^{m,\Delta} - G\|_2 \\
+ \int_0^t \left( C_5(n,s) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m,\Delta}) + C_6(n,s)\|G^{m,\Delta} - G\|_2 \right) C_4(n,s)e_{t,s} C_4(n,r) dr ds \\
\leq C_5(n,t) \left( 1 + \int_0^t C_4(n,s)e_{t,s} C_4(n,r) dr ds \right) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}) \\
+ C_6(n,t) \left( 1 + \int_0^t C_4(n,s)e_{t,s} C_4(n,r) dr ds \right)\|G^{m,\Delta} - G\|_2 \\
= : C_7(n,t) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}) + C_8(n,t)\|G^{m,\Delta} - G\|_2,
\]

which also implies that
\[
W_1(\mu_{t,\Delta}, \mu_{t,\Delta}) \leq C_7(n,t) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}) + C_8(n,t)\|G^{m,\Delta} - G\|_2.
\]
and
\[ \sup_{k \in [n]} |f_t^m(x_k) - f_t(x_k)| \leq (M_\sigma + C_1(n,t)\sigma) \left( C_\tau(n,t) \mathcal{W}_1(\mu_0^m, \mu_0) + C_8(n,t)\|G^m - G\|_2 \right). \]

**E Proof of Lemma 9**

For each \( t \geq 0 \), we write \( \mu_{t,\Delta} = (\dot{e}_{x_1, \ldots, x_n, x'_1, \ldots, x'_{n'}})\#\mu_t^m \) and \( \mu_{t,\Delta}^\ast = (\dot{e}_{x_1, \ldots, x_n, x'_1, \ldots, x'_{n'}})\#\mu_t^m \).

It is straightforward to show that we can write \( \mu_{t,\Delta} = (\Theta_t^\Delta)#(\mu_{0,\Delta}) \) and \( \mu_{t,\Delta}^\ast = (\Theta_{t,\Delta}^\ast)#(\mu_{0,\Delta}^\ast) \), where \( \Theta_t^\Delta = [A_t^\Delta, U_t^\Delta, V_t^\Delta] : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \) and \( \Theta_{t,\Delta}^\ast = [A_{t,\Delta}^\ast, U_{t,\Delta}^\ast, V_{t,\Delta}^\ast] : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \) are defined by, \( \forall a \in \mathbb{R}, u \in \mathbb{R}^n, v \in \mathbb{R}^n \),

\[
A_t^\Delta(a, u, v) = A_t^\Delta(a, u),
A_{t,\Delta}^\ast(a, u, v) = A_{t,\Delta}^\ast(a, u),
U_t^\Delta(a, u, v) = U_t^\Delta(a, u),
U_{t,\Delta}^\ast(a, u, v) = U_{t,\Delta}^\ast(a, u),
\]

and for all \( k' \in [n'] \),

\[
\frac{d}{dt} V_{t,k'}^\Delta(a, u, v) = -\frac{1}{n} A_t^\Delta(a, u) \sum_{k=1}^{n} \sigma'(U_{t,k}^\Delta(a, u))(f_t(x_k) - y_k) G(x_k, x_k'),
\]

\[
\frac{d}{dt} V_{t,k'}^{m,\Delta}(a, u, v) = -\frac{1}{n} A_{t,\Delta}^\ast(a, u) \sum_{k=1}^{n} \sigma'(U_{t,k}^{m,\Delta}(a, u))(f_{m,\Delta}(x_k) - y_k) G(x_k, x_k'),
\]

with \( V_0^\Delta(a, u, v) = V_0^{m,\Delta}(a, u, v) = v \).

Define \( \tilde{\mu}_{t,\Delta}^m = (\Theta_t^\Delta)#\mu_{0,\Delta}^m \). By the triangle inequality,

\[
\mathcal{W}_1(\mu_{t,\Delta}^m, \mu_{t,\Delta}) \leq \mathcal{W}_1(\mu_{t,\Delta}, \tilde{\mu}_{t,\Delta}^m) + \mathcal{W}_1(\tilde{\mu}_{t,\Delta}^m, \mu_{0,\Delta}).
\]

For the first term on the right-hand side,

\[
\mathcal{W}_1(\mu_{t,\Delta}, \tilde{\mu}_{t,\Delta}^m) \leq \text{Lip}(\Theta_t^\Delta) \mathcal{W}_1(\mu_{0,\Delta}, \tilde{\mu}_{0,\Delta}^m) \leq C_9(n,t) \mathcal{W}_1(\mu_{0,\Delta}, \mu_{0,\Delta}^m).
\]

For the second term, we observe that

\[
\mathcal{W}_1(\tilde{\mu}_{t,\Delta}^m, \mu_{0,\Delta}) \leq \int_{\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^{n'}} \|\Theta_t^{m,\Delta}(a, u, v) - \Theta_t^\Delta(a, u, v)\|_2 \mu_{0,\Delta}^m(da, du, dv)
\]

\[
\leq \Delta A_{t,\Delta}^m + \Delta U_{t,\Delta}^m + \Delta V_{t,\Delta}^m,
\]

where we define

\[
\Delta A_{t,\Delta}^m = \int_{\mathbb{R} \times \mathbb{R}^n} |A_{t,\Delta}^m(a, u, v) - A_t^\Delta(a, u, v)| \mu_{t,\Delta}^m(da, du),
\]

\[
\Delta U_{t,\Delta}^m = \int_{\mathbb{R} \times \mathbb{R}^n} \|U_{t,\Delta}^m(a, u, v) - U_{t,\Delta}^\ast(a, u, v)\|_1 \mu_{t,\Delta}^m(da, du),
\]

\[
\Delta V_{t,\Delta}^m = \int_{\mathbb{R} \times \mathbb{R}^n} \|V_{t,\Delta}^m(a, u, v) - V_{t,\Delta}^\ast(a, u, v)\|_1 \mu_{t,\Delta}^m(da, du),
\]

\[
= \int_{\mathbb{R} \times \mathbb{R}^n} \sum_{k=1}^{n} |V_{t,k}^{m,\Delta}(a, u, v) - V_{t,k}^{\ast}(a, u, v)| \mu_{t,\Delta}^m(da, du).
\]
With the definitions in (54), we see that
\[ \Delta A_t^{m,\Delta} = \Delta A_t^{m,\Delta}, \quad \Delta U_t^{m,\Delta} = \Delta U_t^{m,\Delta}, \]
and hence, (53) implies that
\[ \Delta A_t^{m,\Delta} + \Delta U_t^{m,\Delta} \leq C_7(n,t) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + C_8(n,t) \| G_{m_1} - G_{m_2} \| . \]
Moreover, (55) implies that
\[
\int_{\mathbb{R} \times \mathbb{R}^n} \left| \frac{d}{dt} \left( V_{t,k'}^{m,\Delta}(a, u, v) - V_{t,k}^{m,\Delta}(a, u, v) \right) \right| \mu_t^m(da, du) \\
\leq \int_{\mathbb{R} \times \mathbb{R}^n} \left( |A_t^{m,\Delta}(a, u) - A_t^{m,\Delta}(a, u)| \sum_{k=1}^n |\sigma'((U_{t,k}^{m,\Delta}(a, u))| |(f_i(x_k) - y_k)| |G(x_k, x_k')| \\
+ |A_t^{m,\Delta}(a, u)| \sum_{k=1}^n |\sigma'((U_{t,k}^{m,\Delta}(a, u))| |(f_i(x_k) - y_k)| |G(x_k, x_k')| \\
+ |A_t^{m,\Delta}(a, u)| \sum_{k=1}^n |\sigma'((U_{t,k}^{m,\Delta}(a, u))| |(f_i(x_k) - y_k) - (f_i^m(x_k) - y_k)| |G(x_k, x_k')| \\
+ |A_t^{m,\Delta}(a, u)| \sum_{k=1}^n |\sigma'((U_{t,k}^{m,\Delta}(a, u))| |(f_i^m(x_k) - y_k)| |G(x_k, x_k') - G(x_k, x_k')| \right) \mu_t^m(da, du) \\
\leq nL_\sigma(M_\sigma)^2(C_2(n,t) + \| y \|_\infty) \Delta A_t^{m,\Delta} \\
+ L_\sigma(M_\sigma)^2 C_1(n,t)(C_2(n,t) + \| y \|_\infty) \Delta U_t^{m,\Delta} \\
+ nL_\sigma(M_\sigma)^2 C_1(n,t)(M_\sigma + C_1(n,t)L_\sigma)(C_3(n,t) W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + \Delta A_t^{m,\Delta} + \Delta U_t^{m,\Delta}) \\
+ \sqrt{n}L_\sigma C_1(n,t)(C_2(n,t) + \| y \|_\infty) \sum_{k=1}^n |G_{m_1}(x_k, x_k') - G(x_k, x_k')| .
\]
Thus, together with (53), we see there exists a function $C_9'(n,t)$ that is non-negative and non-decreasing in $t$ such that
\[
\Delta V_t^{m,\Delta} \leq \int_0^t C_9(n,s)(\Delta A_s^{m,\Delta} + \Delta U_s^{m,\Delta} + W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + \| G_{m_1} - G_{m_2} \| ) ds \\
\leq \int_0^t C_{10}(n,s)(1 + C_7(n,s) + C_8(n,s))(W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + \| G_{m_1} - G_{m_2} \| ) ds \\
\leq e^{C_9'(n,s)}(1 + C_7(n,s) + C_8(n,s)) ds (W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + \| G_{m_1} - G_{m_2} \| ) \\
= : C_{11}(n,t)(W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + \| G_{m_1} - G_{m_2} \| ) .
\]
Therefore,
\[
W_1(\mu_{\Delta,\Delta}, \mu_{\Delta,\Delta}) \leq C_9(n,t)W_9(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + C_{11}(n,t)(W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + \| G_{m_1} - G_{m_2} \| ) \\
\leq 2C_{11}(n,t)(W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) + \| G_{m_1} - G_{m_2} \| ) ,
\]
since $W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m}) \leq W_1(\mu_{0,\Delta}, \mu_{0,\Delta}^{m})$. 

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We see that

With the value of \( \hat{a} > 0 \) to be specified later, we define \( \xi_{\max} = \min\{\frac{1}{2}(I_r - I_l), \frac{1}{2} \hat{a}\} \) if \( \alpha = \frac{1}{2} \) and \( \min\{\frac{1}{2}I_r, \frac{1}{2}I_l, \frac{1}{2} \hat{a}\} \). We choose any \( \xi \in (0, \xi_{\max}) \) and define an open interval \( I_\xi = (I_l + \xi, I_r - \xi) \).

For each \( k \in [n] \), we define sets \( \Xi, \Xi^\dagger_k \in \mathbb{R} \times \mathcal{C} \) as

\[
\Xi_k = \left\{ a \in \mathbb{R}, h \in \mathcal{C} : |a| \geq \frac{1}{2} \hat{a}, h(x_k) \in I \right\},
\]

\[
\Xi^\dagger_k = \left\{ a \in \mathbb{R}, h \in \mathcal{C} : |a| \geq \frac{1}{2} \hat{a} + \xi, h(x_k) \in I_\xi \right\}.
\]

We see that

\[
-\frac{d}{dt} \mathcal{L}_t \geq \int_{\mathbb{R} \times \mathcal{C}} \frac{(A_t(a,h))^2}{n^2} \sum_{k,l=1}^{n} \sigma'(H_t(a,h)(x_k)) \sigma'(H_t(a,h)(x_l)) (f_t(x_k) - y_k) (f_t(x_l) - y_l) G_{kl} \mu_0(da, dh)
\]

\[
\geq \int_{\mathbb{R} \times \mathcal{C}} \frac{(A_t(a,h))^2}{n^2} \lambda_{\min} \sum_{k=1}^{n} \left( \sigma'(H_t(a,h)(x_k)) \right)^2 (f_t(x_k) - y_k)^2 \mu_0(da, dh)
\]

\[
\geq \frac{\lambda_{\min}(G)}{n^2} \sum_{k=1}^{n} \int_{\Xi_k} \lambda_{\min} \left( \sigma'(H_t(a,h)(x_k)) \right)^2 (f_t(x_k) - y_k)^2 \mu_0(da, dh)
\]

\[
\geq \frac{(K_{\sigma'})^2 \lambda_{\min}(G)}{2n} \hat{a}^2 \left( \min_{k \in [n]} \mu_t(\Xi_k) \right) \mathcal{L}_t.
\]

(58)

In the following lemma, we provide a lower bound on the term \( \min_{k \in [n]} \mu_t(\Xi_k) \) for \( t \geq 0 \) via a fine-grained analysis of the dynamics:

**Lemma 27.** \( \forall t \geq 0, \forall \hat{a} > 0, \)

\[
\min_{k \in [n]} \mu_t(\Xi_k) \geq \left( \min_{k \in [n]} \mu_0(\Xi_k) \right)^{\frac{3}{2}} - \frac{K_1}{\hat{a}^2},
\]

(59)

where \( K_1 = \frac{3(2(\beta_a)^{\frac{1}{2}} + (G_{\max})^{\frac{1}{2}})\|y\|_2}{(\xi(\lambda_{\min}(G))^{\frac{1}{2}})(K_{\sigma'})} \).

This lemma is proved in Appendix F.1, and it extends similar results provided in [11] for the non-asymptotic setting restricted to having \( \beta_a = 0 \) and \( \alpha = \frac{1}{2} \).

By assumption, \( \rho_a((\infty, \hat{a}) \cup (\hat{a}, \infty)) > 0 \). When \( \alpha > \frac{1}{2} \), if Assumptions 2 and 13 are satisfied, we know that for any \( k \in [n] \), \( \mu_0(\Xi^\dagger_k) = \rho_a((-\infty, \frac{1}{2} \hat{a} - \xi) \cup \frac{1}{2} \hat{a} + \xi, \infty)) \geq 2 \rho_a(\hat{a}, \infty) > 0 \). When \( \alpha = \frac{1}{2} \), for any \( k \in [n] \), since \( (e_{x_k})^\# \mu_0 = \mathcal{N}(0, G_{kk}) \), we know that

\[
\mu_0(\Xi^\dagger_k) = \rho_a((-\infty, \frac{1}{2} \hat{a} - \xi) \cup \frac{1}{2} \hat{a} + \xi, \infty)) \int_{I_r - \xi}^{I_l + \xi} \frac{1}{\sqrt{2\pi G_{kk}}} e^{-\frac{u^2}{2G_{kk}}} du
\]

\[
\geq \sqrt{2} \rho_a(\hat{a}, \infty) \frac{I_r - I_l - 2 \xi}{\sqrt{\pi M_{\sigma}}} e^{-\frac{\max(I_r^2, I_l^2)}{e_{\min}^2}} > 0.
\]

Thus, defining

\[
K_2 = \begin{cases} 2 \rho_a(\hat{a}, \infty), & \text{if } \alpha > \frac{1}{2} \\ \sqrt{2} \rho_a(\hat{a}, \infty) \frac{I_r - I_l - 2 \xi}{\sqrt{\pi M_{\sigma}}} e^{-\frac{\max(I_r^2, I_l^2)}{e_{\min}^2}}, & \text{if } \alpha = \frac{1}{2} \end{cases},
\]

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it holds that \(\min_{k \in [n]} \mu_0(\Xi_k) > K_2 > 0\). Hence, if we choose \(\hat{a} \geq 4K_1/(3K_2)^{\frac{3}{2}}\), then \(\forall t \geq 0\),

\[
\min_{k \in [n]} \mu_t(\Xi_k) \geq \left(\frac{1}{4}(K_2)^{\frac{3}{2}}\right)^{\frac{3}{2}} = \frac{1}{8}K_2 > 0.
\]

This allows us to conclude that

\[
- \frac{d}{dt} \mathcal{L}_t \geq \frac{\lambda_{\min}(G)(K_\sigma)^2\hat{a}^2}{2n}K_2 \mathcal{L}_t,
\]

and hence \(\mathcal{L}_t \leq \mathcal{L}_0 e^{-r\lambda_{\min} \hat{a}^2 t}\), where \(r = (K_\sigma)^2K_2/(2n)\).

### F.1 Proof of Lemma 27

We first prove a relevant lemma about the dynamics of \(A_t\) and \(H_t\).

**Lemma 28.** \(\forall t \geq 0\),

\[
\int_{\mathbb{R} \times C} \left| \frac{d}{dt} A_t(a, h) \right|^2 \mu_0(da, dh) \leq -\beta \frac{d}{dt} \mathcal{L}_t,
\]

and \(\forall x \in \mathcal{X}',\)

\[
\int_{\mathbb{R} \times C} \left| \frac{d}{dt} H_t(a, h)(x) \right|^2 \mu_0(da, dh) \leq -G_{\max} \frac{d}{dt} \mathcal{L}_t.
\]

**Proof** For \(t \geq 0, a \in \mathbb{R}, h \in C\), define a function \(g_t(\cdot; a, h)\) on \(\mathbb{R}^d\) by, \(\forall z \in \mathbb{R}^d\),

\[
g_t(z; a, h) = -\frac{1}{n} A_t(a, h) \sum_{k=1}^n \sigma'(H_t(a, h)(x_k))(f_t(x_k) - y_k)\sigma(z^\top x_k).
\]

On one hand, there is \(\frac{d}{dt} H_t(a, h)(x) = \int_{\mathbb{R}^d} g_t(z; a, h)\sigma(z^\top x)\rho_z(dz)\), and so \(\forall x \in \mathcal{X}'\), by the Cauchy-Schwartz inequality,

\[
\left| \frac{d}{dt} H_t(a, h)(x) \right| \leq \left(\int_{\mathbb{R}^d} (g_t(z; a, h))^2 \rho_z(dz)\right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^d} (\sigma(z^\top x))^2 \rho_z(dz)\right)^{\frac{1}{2}}
\]

\[
\leq \left( G_{\max} \int_{\mathbb{R}^d} (g_t(z; a, h))^2 \rho_z(dz)\right)^{\frac{1}{2}}.
\]

On the other hand, we see that

\[
\int_{\mathbb{R}^d} |g_t(z; a, h)|^2 \rho_z(dz)
\]

\[
= \int_{\mathbb{R}^d} \frac{1}{n^2} |A_t(a, h)|^2 \sum_{k, l=1}^n \sigma'(H_t(a, h)(x_k)) \sigma'(H_t(a, h)(x_l))(f_t(x_k) - y_k)(f_t(x_l) - y_l)\sigma(z^\top x_k)\sigma(z^\top x_l)\rho_z(dz)
\]

\[
= \frac{1}{n^2} |A_t(a, h)|^2 \sum_{k, l=1}^n \sigma'(H_t(a, h)(x_k)) \sigma'(H_t(a, h)(x_l))(f_t(x_k) - y_k)(f_t(x_l) - y_l)G_{kl}
\]

and hence

\[
- \frac{d}{dt} \mathcal{L}_t = \int_{\mathbb{R} \times C} \frac{\beta}{n^2} \sum_{k, l=1}^n (f_t(x_k) - y_k)(f_t(x_l) - y_l)\sigma(H_t(a, h)(x_k)) \sigma(H_t(a, h)(x_l)) \mu_0(da, dh)
\]

\[
+ \int_{\mathbb{R} \times C} \frac{1}{n^2} |A_t(a, h)|^2 \sum_{k, l=1}^n \sigma'(H_t(a, h)(x_k)) \sigma'(H_t(a, h)(x_l))(f_t(x_k) - y_k)(f_t(x_l) - y_l)G_{kl}\mu_0(da, dh)
\]

\[
= \beta^{-1} \int_{\mathbb{R} \times C} \left| \frac{d}{dt} A_t(a, h) \right|^2 \mu_0(da, dh) + \int_{\mathbb{R} \times C} \int_{\mathbb{R}^d} |g_t(z; a, h)|^2 \rho_z(dz)\mu_0(da, dh).
\]
Thus,
\[
\int_{\mathbb{R} \times C} \left| \frac{d}{dt} A_t(a, h) \right|^2 \mu_0(da, dh) \leq - \frac{\beta}{dt} L_t,
\]
and by (62), we know that \( \forall x \in X \),
\[
\int_{\mathbb{R} \times C} \left| \frac{d}{dt} H_t(a, h)(x) \right|^2 \mu_0(da, dh) \leq - \frac{G_{\text{max}}}{dt} L_t.
\]

Next, we will prove Lemma 27. Since \( \forall k \in [n] \), \( \forall t \geq 0 \), there is
\[
\Xi_k^+ \subseteq (\Theta_t)^{-1}(\Xi_k) \cup \{ a \in \mathbb{R}, h \in C : |A_t(a, h) - a| > \xi \}
\]
\[
\cup \{ a \in \mathbb{R}, h \in C : |H_t(a, h)(x_k) - h(x_k)| > \xi \},
\]
we know that
\[
\mu_0(\Xi_k^+) \leq \mu_t(\Xi_k) + \mu_0(\{ a \in \mathbb{R}, h \in C : |A_t(a, h) - a| > \xi \})
\]
\[
+ \mu_0(\{ a \in \mathbb{R}, h \in C : |H_t(a, h)(x_k) - h(x_k)| > \xi \}).
\]
Meanwhile, we know that
\[
\int_{\mathbb{R} \times C} |A_t(a, h) - a| \mu_0(da, dh) \leq \int_{\mathbb{R} \times C} \int_0^t \left| \frac{d}{ds} A_s(a, h) \right| ds \mu_0(da, dh)
\]
\[
\leq \int_0^t \left( \int_{\mathbb{R} \times C} \left| \frac{d}{ds} A_s(a, h) \right|^2 \mu_0(da, dh) \right)^{1/2} ds
\]
\[
\leq (\beta_a)^{1/2} \int_0^t \left( - \frac{d}{ds} L_s \right)^{1/2} ds,
\]
and \( \forall k \in [n] \),
\[
\int_{\mathbb{R} \times C} |H_t(a, h)(x_k) - h(x_k)| \mu_0(da, dh) \leq \int_{\mathbb{R} \times C} \int_0^t \left| \frac{d}{ds} H_s(a, h)(x_k) \right| ds \mu_0(da, dh)
\]
\[
\leq \int_0^t \left( \int_{\mathbb{R} \times C} \left| \frac{d}{ds} H_s(a, h)(x_k) \right|^2 \mu_0(da, dh) \right)^{1/2} ds
\]
\[
\leq (G_{\text{max}})^{1/2} \int_0^t \left( - \frac{d}{ds} L_s \right)^{1/2} ds.
\]
Thus, by Markov’s inequality,
\[
\mu_0(\{ a \in \mathbb{R}, h \in C : |A_t(a, h) - a| > \xi \}) \leq \xi^{-1} \int_{\mathbb{R} \times C} |A_t(a, h) - a| \mu_0(da, dh)
\]
\[
\leq \frac{(\beta_a)^{1/2}}{\xi} \int_0^t \left( - \frac{d}{ds} L_s \right)^{1/2} ds,
\]
and $\forall k \in [n]$,

$$\mu_0 \{ \{ a \in \mathbb{R}, h \in C : |H_t(a, h)(x_k) - h(x_k)| > \xi \} \} \leq \xi^{-1} \int_{\mathbb{R} \times C} |H_t(a, h)(x_k) - h(x_k)| \mu_0(da, dh) \leq (\mathcal{G}_{\text{max}})^{\frac{1}{2}} \xi \int_0^t \left( -\frac{d}{ds} \mathcal{L}_s \right)^{\frac{1}{2}} ds.$$ 

Hence, $\forall k \in [n]$,

$$\mu_t(\Xi_k) \geq \mu_0(\Xi_k^+) - \frac{(\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi} \int_0^t \left( -\frac{d}{ds} \mathcal{L}_s \right)^{\frac{1}{2}} ds.$$

Thus, defining $\eta_t = \min_{k \in [n]} \mu_0(\Xi_k^+) - \frac{(\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi} \int_0^t \left( -\frac{d}{ds} \mathcal{L}_s \right)^{\frac{1}{2}} ds$, we have $\min_{k \in [n]} \mu_t(\Xi_k) \geq \eta_t$. Therefore, via (58), we deduce that

$$-\frac{d}{dt} \eta_t = \frac{(\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi} \left( -\frac{d}{dt} \mathcal{L}_t \right)^{\frac{1}{2}}.$$

On the other hand, the definition of $\eta_t$ implies that

$$-\frac{d}{dt} \eta_t = \frac{\lambda_{\text{min}}(K_{\sigma'})^2 \hat{a}^2}{2n} \eta_t \mathcal{L}_t.$$

Combined together, they imply that

$$-\frac{d}{dt} \eta_t = \frac{(\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi} \left( -\frac{d}{dt} \mathcal{L}_t \right)^{-\frac{1}{2}} \leq \frac{(\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi} \left( -\frac{d}{dt} \mathcal{L}_t \right)^{-\frac{1}{2}} \left( \frac{\lambda_{\text{min}}(K_{\sigma'})^2 \hat{a}^2}{2n} \eta_t \mathcal{L}_t \right)^{\frac{1}{2}} \leq \frac{(\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi (\lambda_{\text{min}}(G))^\frac{1}{2} K_{\sigma'} \hat{a}} \left( \eta_t \right)^{-\frac{1}{2}} \left( \mathcal{L}_t \right)^{-\frac{1}{2}} \left( -\frac{d}{dt} \mathcal{L}_t \right)^{\frac{1}{2}}.$$

Therefore,

$$\frac{d}{dt} \left( \frac{2}{3} (\eta_t)^{\frac{3}{2}} \right) = (\eta_t)^{-\frac{1}{2}} \frac{d}{dt} \eta_t \geq \frac{(\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi (\lambda_{\text{min}}(G))^\frac{1}{2} K_{\sigma'} \hat{a}} \left( \eta_t \right)^{-\frac{1}{2}} \left( \mathcal{L}_t \right)^{-\frac{1}{2}} \frac{d}{dt} \left( 2(\mathcal{L}_t)^{\frac{1}{2}} \right),$$

which implies that

$$\frac{2}{3} (\eta_t)^{\frac{3}{2}} \geq \frac{2}{3} (\eta^0)^{\frac{3}{2}} + \frac{2\sqrt{2} (\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi (\lambda_{\text{min}}(G))^\frac{1}{2} K_{\sigma'} \hat{a}} \left( \mathcal{L}_0 \right)^{\frac{1}{2}} \left( \eta_t \right)^{-\frac{1}{2}} \left( \mathcal{L}_t \right)^{-\frac{1}{2}} \frac{d}{dt} \left( 2(\mathcal{L}_t)^{\frac{1}{2}} \right)$$

$$\geq \frac{2}{3} \min_{k \in [n]} \mu_0(\Xi_k)^{\frac{3}{2}} + \frac{2\sqrt{2} (\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\text{max}})^{\frac{1}{2}}}{\xi (\lambda_{\text{min}}(G))^\frac{1}{2} K_{\sigma'} \hat{a}} \left( \mathcal{L}_0 \right)^{\frac{1}{2}},$$

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and hence

\[
\min_{k \in [n]} \mu_{\tau}(\Xi_k) \geq \eta_{\tau} \geq \left( \frac{\min_{k \in [n]} \mu_0(\Xi_k)}{a} \right) \frac{C}{\xi} \lambda_{\min}(G) \frac{1}{K_{\sigma'}} \frac{1}{K_{\sigma'}},
\]

where we define

\[
C = \frac{3\sqrt{2} \left( (\beta_a)^{\frac{1}{2}} + (\mathcal{G}_{\max})^{\frac{1}{2}} \right) n^{\frac{1}{2}} (\tilde{\mathcal{L}}_0)^{\frac{1}{2}}}{\xi(\lambda_{\min}(G))^{\frac{1}{2}} K_{\sigma'}},
\]

where \( \lambda_{\min}(G) \) is the minimum eigenvalue of the matrix \( G \).

**G Proof of Lemma 15**

It follows from (62) and the results in [6] that \( \left\| \frac{d}{dt} H_t(a, h) \right\|_H^2 = \int_{\mathcal{H}} |g_t(z; a, h)|^2 \rho_z(dz) \). Thus, the first bound in Lemma 15 follows from (64), and the second bound follows from a direct upper bound of the right-hand-side of (61) together with (60).

**H Proof of Lemma 16**

Using “sup_\mu” as a shorthand for taking the supremum over all \( \mu \in \mathcal{P}(\mathbb{R} \times \mathcal{U}) \) such that \( \int_{\mathbb{R} \times \mathcal{U}} |a| h \mu(da, dh) \leq \kappa \), we have

\[
\hat{\text{Rad}}_S(\mathcal{F}(\mathcal{U}, \kappa)) = \frac{1}{n} \mathbb{E}_r \left[ \sup_{\mu} \sum_{k=1}^n \tau_k \int_{\mathbb{R} \times \mathcal{U}} a \sigma(h(x_k)) \mu(da, dh) \right]
\]

\[
= \frac{1}{n} \mathbb{E}_r \left[ \sup_{\mu} \int_{\mathbb{R} \times \mathcal{U}} \sum_{k=1}^n \tau_k \frac{a \sigma(h(x_k))}{h} \mu(da, dh) \right]
\]

\[
\leq \frac{\kappa}{n} \mathbb{E}_r \left[ \sup_{a \in \mathcal{U}, h \in \mathcal{U}} \sum_{k=1}^n \tau_k \frac{a \sigma(h(x_k))}{h} \right]
\]

\[
\leq \frac{\kappa}{n} \mathbb{E}_r \left[ \sup_{h \in \mathcal{B}(\mathcal{U}, 1)} \sum_{k=1}^n \tau_k \sigma(h(x_k)) \right],
\]

where for the last line, we use the 1-homogeneity of \( \sigma \), which implies that for any \( h \in \mathcal{U} \setminus \{0\} \), \( h/\|h\|_U \) belongs to \( \mathcal{B}(\mathcal{U}, 1) \) and satisfies \( \forall x \in \mathcal{X}, (h/\|h\|_U)(x) = h(x)/\|h\|_U \).

Moreover, the 1-homogeneity of \( \sigma \) also implies that \( \sigma(0) = 0 \). Thus, since \( 0 \in \mathcal{B}(\mathcal{U}, 1) \), we have \( \sup_{h \in \mathcal{B}(\mathcal{U}, 1)} \sum_{k=1}^n \tau_k \sigma(h(x_k)) = \left| \sup_{h \in \mathcal{B}(\mathcal{U}, 1)} \sum_{k=1}^n \tau_k \sigma(h(x_k)) \right| \geq 0 \). Therefore,

\[
\hat{\text{Rad}}_S(\mathcal{F}(\mathcal{U}, \kappa)) = \frac{\kappa}{n} \mathbb{E}_r \left[ \sup_{h \in \mathcal{B}(\mathcal{U}, 1)} \sum_{k=1}^n \tau_k \sigma(h(x_k)) \right]
\]

\[
\leq \frac{L_{\sigma} \kappa}{n} \mathbb{E}_r \left[ \sup_{h \in \mathcal{B}(\mathcal{U}, 1)} \sum_{k=1}^n \tau_k \hat{h}(x_k) \right]
\]

\[
= L_{\sigma} \kappa \hat{\text{Rad}}_S(\mathcal{B}(\mathcal{U}, 1)),
\]

where for the second line, we use Lemma 29 with \( \Phi_k(u) = \sigma(u), \forall k \in [n] \).
Lemma 29 (Ledoux-Talagrand contraction lemma). Suppose $F$ is any function class and for each $k \in [n]$, $\Phi_k$ is an $L$-Lipschitz function. Then

$$\frac{1}{n} \mathbb{E}_F \left[ \sup_{h \in F} \sum_{k=1}^n \tau_k(\Phi_k \circ h)(x_k) \right] \leq \frac{L}{n} \mathbb{E}_F \left[ \sup_{h \in F} \sum_{k=1}^n \tau_k h(x_k) \right].$$

A proof can be found in Mohri et al. [52], while a similar result appears in Ledoux and Talagrand [41].

Thus,

$$\text{Rad}_n(F(U, \kappa)) = \mathbb{E}_{S \sim \mathcal{D}^n} \left[ \text{Rad}_S(F(U, \kappa)) \right] \leq L_\sigma \kappa \mathbb{E}_{S \sim \mathcal{D}^n} \left[ \text{Rad}_S(B(U, 1)) \right] = L_\sigma \kappa \text{Rad}_n(B(U, 1)).$$

I Proof of Lemma 18

We will state and prove a more general version of Lemma 18 that is also applicable when $\beta_a > 0$. First, we extend the definition of the norm $\gamma^p_a$ to include the case $\beta_a > 0$ as follows. We define the following norm (or extended norm) on $\mathbb{R} \times \mathcal{U}$ (or $\mathbb{R} \times \mathcal{C}$):

$$\| (a, h) \| = \max \{ C_{\beta_a} |a|, \|h\|_U \},$$

where $C_{\beta_a} \in [0, \infty]$ is a constant to be specified that depends on $\beta_a$. This norm (or extended norm) induces an metric (or extended metric) on $\mathbb{R} \times \mathcal{U}$ (or $\mathbb{R} \times \mathcal{C}$): $\forall a_1, a_2 \in \mathbb{R}$ and $\forall h_1, h_2 \in \mathcal{U}$ (or $\mathcal{C}$),

$$d((a_1, h_1), (a_2, h_2)) = \| (a_1 - a_2, h_1 - h_2) \|.$$

Then, we can define extended Wasserstein distances between probability measures on $\mathbb{R} \times \mathcal{C}$ as follows. Let $\mu, \mu'$ be two probability measures on $\mathbb{R} \times \mathcal{C}$, and let $\mathcal{J}(\mu, \mu')$ denote the space of probability measures on $(\mathbb{R} \times \mathcal{C}) \times (\mathbb{R} \times \mathcal{C})$ with marginals equal to $\mu$ and $\mu'$, respectively. For $p \in [1, \infty)$, we define the $p$-Wasserstein-like distance between $\mu$ and $\mu'$ by

$$W_p(\mu, \mu'; \mathcal{U}) = \left( \inf_{\pi \in \mathcal{J}(\mu, \mu')} d((a_1, h_1), (a_2, h_2))^p \pi(da_1, dh_1, da_2, dh_2) \right)^{\frac{1}{p}},$$

and moreover,

$$W_\infty(\mu, \mu'; \mathcal{U}) = \inf_{\pi \in \mathcal{J}(\mu, \mu')} \sup((a_1, h_1), (a_2, h_2)) \in \text{supp}(\pi) d((a_1, h_1), (a_2, h_2)).$$

When $\beta_a = 0$, we set $C_{\beta_a} = \infty$. Thus, under the convention “$0 \cdot \infty = 0$”, we see that (66) and (67) are equivalent to the definitions (31) and (32). Thus, we state the following lemma, which extends Lemma 18.

Lemma 30. Assume that $\sigma$ is $L_\sigma$-Lipschitz with $L_\sigma > 0$ and $\int_{\mathbb{R} \times \mathcal{C}} |a| \mu_{\text{base}}(da, dh) = \bar{a} < \infty$. If $\beta_a > 0$, we further assume that $|\sigma(u)| < M_\sigma$, $\forall u \in \mathbb{R}$. Then,

$$\text{Rad}_n(\mathcal{F}_\infty^+(U, \mu_{\text{base}}, \kappa)) \leq (G_{\text{max}})^{\frac{1}{2}} L_\sigma \left( \bar{a} + \frac{\kappa}{C_{\beta_a}} \right)^{\frac{\kappa}{\sqrt{n}}} + \frac{L_\sigma M_\sigma}{C_{\beta_a}} \frac{\kappa^2}{\sqrt{n}}.$$
**Proof** Given any \( f \in \mathcal{F}^+_\infty(\mathcal{U}, \mu_{\text{base}}, \kappa) \), let \( \mu \) denote its corresponding measure. Define the function \( f_{\text{base}}(x) = \int_{\mathbb{X}} \sigma(h(x)) \mu_{\text{base}}(da, dh) \) on \( \mathcal{X} \). Since \( \mathcal{W}_{\infty}(\mu_{\text{base}}, \mu; \mathcal{U}) < \kappa \), we know that \( \exists \pi \in \hat{\mathcal{J}}(\mu_{\text{base}}, \mu) \) such that \( \forall ((a_1, h_1), (a_2, h_2)) \in \text{supp}(\pi), \)
\[
d((a_1, h_1), (a_2, h_2)) \leq \kappa.
\] (68)

We then see that
\[
f(x) = \int_{\mathbb{X}} a_{\ast} \sigma(h_{\ast}(x)) \mu(da_{\ast}, dh_{\ast})
\]
\[
= \int_{\mathbb{X}} a_{\ast} \sigma(h_{\ast}(x)) \pi(da, dh, da_{\ast}, dh_{\ast})
\]
\[
= \int_{\mathbb{X}} (a + \tilde{a}) \sigma(h(x) + \tilde{h}(x)) \tilde{\pi}(da, dh, d\tilde{a}, d\tilde{h}) ,
\]
where \( \tilde{\pi} \) is the push-forward of \( \pi \) under the map \( (a, h, a', h') \mapsto (a, h, a' - a, h' - h) \). Let \( \xi(da, d\tilde{h}; a, h) \) denote the Radon-Nikodym derivative of \( \tilde{\pi} \) with respect to \( \mu_{\text{base}} \) (or in other words, the conditional probability measure of \( \tilde{a} \) and \( \tilde{h} \) with respect to \( a \) and \( h \)). Then, (68) implies that \( \forall (a, h) \in \text{supp}(\mu_{\text{base}}), \xi(\cdot; a, h) \) is supported on \( B(\mathbb{R} \times \mathcal{U}, \kappa) \), where we define \( B(\mathbb{R} \times \mathcal{U}, \kappa) = \{(a, h) \in \mathbb{R} \times \mathcal{U} : \| (a, h) \| \leq \kappa \} \). Thus,
\[
f(x) = \int_{\mathbb{X}} \int_{\mathbb{X}} (a + \tilde{a}) \sigma(h(x) + \tilde{h}(x)) \xi(da, d\tilde{h}; a, h) \mu_{\text{base}}(da, dh)
\]
\[
= \int_{\mathbb{X}} \int_{B(\mathbb{R} \times \mathcal{U}, \kappa)} (a + \tilde{a}) \sigma(h(x) + \tilde{h}(x)) \xi(da, d\tilde{h}; a, h) \mu_{\text{base}}(da, dh) ,
\]
and
\[
f(x) - f_{\text{base}}(x) = \int_{\mathbb{X}} \left( \int_{B(\mathbb{R} \times \mathcal{U}, \kappa)} (a + \tilde{a}) \sigma(h(x) + \tilde{h}(x)) \xi(da, d\tilde{h}; a, h) - a \sigma(h(x)) \right) \mu_{\text{base}}(da, dh)
\]
\[
= \int_{\mathbb{X}} \int_{B(\mathbb{R} \times \mathcal{U}, \kappa)} ((a + \tilde{a}) \sigma(h(x) + \tilde{h}(x)) - a \sigma(h(x))) \xi(da, d\tilde{h}; a, h) \mu_{\text{base}}(da, dh) .
\]

Given \( S = \{x_1, \ldots, x_n\} \subseteq \mathcal{X} \), the empirical Rademacher complexity of \( \mathcal{F}^+_\infty(\mathcal{U}, \mu_{\text{base}}, \kappa) \) is
\[
\hat{\text{Rad}}_S(\mathcal{F}^+_\infty(\mathcal{U}, \mu_{\text{base}}, \kappa))
\]
\[
= \frac{1}{n} \mathbb{E}_T \left[ \sup_{f \in \mathcal{F}^+_\infty(\mathcal{U}, \mu_{\text{base}}, \kappa)} \sum_{k=1}^{n} \tau_k f(x_k) \right]
\]
\[
= \frac{1}{n} \mathbb{E}_T \left[ \sup_{f \in \mathcal{F}^+_\infty(\mathcal{U}, \mu_{\text{base}}, \kappa)} \sum_{k=1}^{n} \tau_k \left( f(x_k) - f_{\text{base}}(x_k) \right) \right]
\]
\[
= \frac{1}{n} \mathbb{E}_T \left[ \sup_{\xi(\cdot; a, h)} \int_{\mathbb{X}} \int_{\mathbb{X}} \int_{\mathbb{U}} \sum_{k=1}^{n} \tau_k \left( (a + \tilde{a}) \sigma(h(x_k) + \tilde{h}(x_k)) - a \sigma(h(x_k)) \right) \xi(da, d\tilde{h}; a, h) \mu_{\text{base}}(da, dh) \right]
\]
\[
= \frac{1}{n} \mathbb{E}_T \left[ \int_{\mathbb{X}} \sup_{\xi(\cdot; a, h) \in B(\mathbb{R} \times \mathcal{U}, \kappa)} \int_{\mathbb{U}} \sum_{k=1}^{n} \tau_k \left( (a + \tilde{a}) \sigma(h(x_k) + \tilde{h}(x_k)) - a \sigma(h(x_k)) \right) \xi(da, d\tilde{h}; a, h) \mu_{\text{base}}(da, dh) \right]
\]
\[
\leq \int_{\mathbb{X}} \frac{1}{n} \mathbb{E}_T \left[ \sup_{(\tilde{a}, \tilde{h}) \in B(\mathbb{R} \times \mathcal{U}, \kappa)} \sum_{k=1}^{n} \tau_k \left( (a + \tilde{a}) \sigma(h(x_k) + \tilde{h}(x_k)) - a \sigma(h(x_k)) \right) \mu_{\text{base}}(da, dh) \right] .
\]
where in lines 4 - 6, the supremum is taken over all $\xi$ such that $\forall (a, h) \in \text{supp}(\mu_{\text{base}})$, $\xi(\cdot, \cdot; a, h)$ is supported in $\mathcal{P}(B(\mathbb{R} \times \mathcal{U}, \kappa))$. For each $a \in \mathbb{R}$ and $h \in \mathcal{C}$, we see that

$$1\ E_\tau \left[ \frac{1}{n} \sup_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} \tau_k \left( (a + \hat{a}) \sigma(h(x_k)) + \tilde{h}(x_k) - a \sigma(h(x_k)) \right) \right]$$

$$\leq 1\ E_\tau \left[ \frac{1}{n} \sum_{\| \hat{a}, \hat{h} \| \leq \kappa} \tau_k a \left( \sigma(h(x_k)) + \tilde{h}(x_k) - \sigma(h(x_k)) \right) \right]$$

$$+ \frac{1}{n} \ E_\tau \left[ \sup_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} \tau_k \tilde{a} \left( \sigma(h(x_k)) + \tilde{h}(x_k) - \sigma(h(x_k)) \right) \right]$$

$$+ \frac{1}{n} \ E_\tau \left[ \sup_{\| \hat{a} \| \leq \kappa/\beta a} \sum_{k=1}^{n} \tau_k \tilde{a} \sigma(h(x_k)) \right] .$$

We bound the three terms on the right-hand side separately. For the first term,

$$1\ n \ E_\tau \left[ \sup_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} \tau_k a \left( \sigma(h(x_k)) + \tilde{h}(x_k) - \sigma(h(x_k)) \right) \right]$$

$$\leq \left| a \right| \ E_\tau \left[ \sum_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} \tau_k \left( \sigma(h(x_k)) + \tilde{h}(x_k) - \sigma(h(x_k)) \right) \right]$$

$$\leq \left| a \right| \left( \sum_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} \tau_k \left( \sigma(h(x_k)) + \tilde{h}(x_k) - \sigma(h(x_k)) \right) \right)$$

$$+ 2\left| a \right| \ E_\tau \left[ \sum_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} (-\tau_k) \left( \sigma(h(x_k)) + \tilde{h}(x_k) - \sigma(h(x_k)) \right) \right]$$

$$\leq L_{\sigma} \left| a \right| \ E_\tau \left[ \sum_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} \tau_k \tilde{h}(x_k) \right]$$

$$= L_{\sigma} \left| a \right| \text{Rad}_{L_2}(B(\mathcal{U}, \kappa)) .$$

where the second inequality uses the fact that $B(\mathcal{U}, \kappa)$ contains the zero function for any $\kappa \geq 0$, which implies that for any $\tau$,

$$\sup_{\| \hat{a}, \hat{h} \| \leq \kappa} \sum_{k=1}^{n} \tau_k \left( \sigma(h(x_k)) + \tilde{h}(x_k) - \sigma(h(x_k)) \right) \geq \sum_{k=1}^{n} \tau_k \left( \sigma(h(x_k)) + 0 - \sigma(h(x_k)) \right) = 0 ;$$

the third inequality uses the symmetry of the Rademacher distribution; and the fourth inequality uses Lemma 29, with each $\Phi_k(u)$ defined to be $\sigma(h(x_k) + u) - \sigma(h(x_k))$. 

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For the second term,
\[
\frac{1}{n} \mathbb{E}_\tau \left[ \sup_{|\hat{a}| \leq \kappa/C_{\beta_a}} \sum_{k=1}^n \tau_k \hat{a} \left( \sigma(h(x_k)) - \tilde{h}(x_k) \right) \right] \leq \frac{1}{n} \mathbb{E}_\tau \left[ \sup_{|\hat{a}| \leq \kappa/C_{\beta_a}} \sum_{k=1}^n \tau_k \hat{a} \left( \sigma(h(x_k)) - \sigma(h(x_k)) \right) \right] \leq \frac{2\kappa}{C_{\beta_a} n} \mathbb{E}_\tau \left[ \sum_{k=1}^n \tau_k \hat{a} \right] \leq \frac{2\kappa}{C_{\beta_a} n} \mathbb{E}_\tau \left[ \sum_{k=1}^n \tau_k \hat{a} \right] \leq \frac{L_\sigma \kappa}{C_{\beta_a}} \mathbb{E}_\tau \left[ \sum_{k=1}^n \tau_k \hat{a} \right] \leq \frac{L_\sigma \kappa}{C_{\beta_a}} \text{Rad}_S(B(\mathcal{U}, \kappa)),
\]
where the third and fourth inequalities again use the fact that $B(\mathcal{U}, \kappa)$ contains the zero function for any $\kappa \geq 0$ and Lemma 29, respectively.

For the third term,
\[
\frac{1}{n} \mathbb{E}_\tau \left[ \sup_{(\hat{a}, \tilde{h}) \in B(\mathbb{R}^d \times \mathbb{R}, \kappa)} \sum_{k=1}^n \tau_k \hat{a} \sigma(h(x_k) + \tilde{h}(x_k)) \right] = \frac{\kappa}{n C_{\beta_a}} \mathbb{E}_\tau \left[ \sum_{k=1}^n \tau_k \sigma(h(x_k)) \right] \leq \frac{\kappa}{n C_{\beta_a}} \left( \mathbb{E}_\tau \left[ \sum_{k=1}^n \tau_k \sigma(h(x_k)) \right]^2 \right)^{\frac{1}{2}} \leq \frac{L_\sigma \kappa}{\sqrt{n C_{\beta_a}}}.
\]

Therefore, from (69) we deduce that
\[
\frac{1}{n} \mathbb{E}_\tau \left[ \sup_{(\hat{a}, \tilde{h}) \in B(\mathbb{R}^d \times \mathbb{R}, \kappa)} \sum_{k=1}^n \tau_k (a + \hat{a}) \sigma(h(x_k) + \tilde{h}(x_k)) \right] \leq \left( L_\sigma |a| + \frac{L_\sigma \kappa}{C_{\beta_a}} \right) \text{Rad}_S(B(\mathcal{U}, \kappa)) + \frac{M_\sigma \kappa}{\sqrt{n C_{\beta_a}}},
\]
Hence,
\[
\text{Rad}_S(F_\infty^+ (U, \mu_{\text{base}}, \kappa)) \leq \int_{\mathbb{R} \times \mathcal{C}} \left( L_\sigma |a| + \frac{L_\sigma \kappa}{C_{\beta_a}} \right) \text{Rad}_S(B(\mathcal{U}, \kappa)) + \frac{M_\sigma \kappa}{\sqrt{n C_{\beta_a}}} \mu_{\text{base}}(da, dh) \leq \frac{L_\sigma \kappa}{C_{\beta_a}} \text{Rad}_S(B(\mathcal{U}, \kappa)) + \frac{M_\sigma \kappa}{\sqrt{n C_{\beta_a}}}.
\]
Since $\text{Rad}_S(B(\mathcal{U}, \kappa)) \leq (G_{\max})^\frac{1}{2} \kappa$, We derive that
\[
\text{Rad}_S(F_\infty^+ (U, \mu_{\text{base}}, \kappa)) \leq (G_{\max})^\frac{1}{2} L_\sigma \left( \frac{L_\sigma \kappa}{C_{\beta_a}} \right) \frac{\kappa}{\sqrt{n}} + \frac{L_\sigma \kappa}{C_{\beta_a}} \frac{\kappa^2}{\sqrt{n}}.
\]
Therefore,
\[
\text{Rad}_n(F_\infty^+ (U, \mu_{\text{base}}, \kappa)) = \mathbb{E}_{S \sim \mathcal{D}^n} \left[ \text{Rad}_S(F_\infty^+ (U, \mu_{\text{base}}, \kappa)) \right] \leq (G_{\max})^\frac{1}{2} L_\sigma \left( \frac{L_\sigma \kappa}{C_{\beta_a}} \right) \frac{\kappa}{\sqrt{n}} + \frac{L_\sigma \kappa}{C_{\beta_a}} \frac{\kappa^2}{\sqrt{n}}.
\]
In particular, when $\beta_a = 0$, the results above reduce to Lemma 18 and Corollary 19 (without requiring $\sigma$ to be bounded).

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