A Quadrature Perspective on Frequency Bias in Neural Network Training with Nonuniform Data

Abstract

Small generalization errors of over-parameterized neural networks (NNs) can be partially explained by the frequency biasing phenomenon, where gradient-based algorithms minimize the low-frequency misfit before reducing the high-frequency residuals. Using the Neural Tangent Kernel (NTK), one can provide a theoretically rigorous analysis for training where data are drawn from constant or piecewise-constant probability densities. Since most training data sets are not drawn from such distributions, we use the NTK model and a data-dependent quadrature rule to theoretically quantify the frequency biasing of NN training given fully nonuniform data. By replacing the loss function with a carefully selected Sobolev norm, we can further amplify, dampen, counterbalance, or reverse the intrinsic frequency biasing in NN training.

1 Introduction

Neural networks (NNs) are often trained in supervised learning on a small data set. They are observed to provide accurate predictions for a large number of test examples that are not seen during training. A mystery is how training can achieve quite small generalization errors in an overparameterized NN and a so-called “double-descent” risk curve [Belkin et al., 2019]. In recent years, a potential answer has emerged called “frequency biasing,” which is the phenomenon that in the early epochs of training, an overparameterized NN finds a low-frequency fit of the training data while higher frequencies are learned in later epochs [Rahaman et al., 2019, Yang and Salman, 2019, Xu, 2020]. Currently, frequency biasing is theoretically understood via the Neural Tangent Kernel (NTK) [Jacot et al., 2018] for uniform training data [Arora et al., 2019, Cao et al., 2019, Basri et al., 2019] and data distributed according to a piecewise constant probability measure [Basri et al., 2020]. However, most training data sets in practice are highly clustered and not uniform. Yet, frequency biasing is still observed during NN training [Fridovich-Keil et al., 2021], even though the theory is absent. This paper proves that frequency biasing is present when there is nonuniform training data by using a new viewpoint based on a data-dependent quadrature rule. We use this theory to propose new loss functions for NN training that accelerate its convergence and improve stability with respect to noise.

A NN function is a map \( N : \mathbb{R}^d \to \mathbb{R} \) given by

\[
N(x) = W_{N_L} \sigma \left( W_{N_L-1} \sigma \left( \cdots \left( W_2 \sigma (W_1 x + b_1) + b_2 \right) + \cdots \right) + b_{N_L-1} \right) + b_{N_L},
\]

where \( W_i \in \mathbb{R}^{m_i \times m_{i-1}} \) are weights, \( m_0 = d, b_i \in \mathbb{R}^{m_i} \) are biases, and \( N_L \) is the number of layers. Here, \( \sigma \) is the activation function and applied entry-wise to a vector, i.e., \( \sigma(a)_j = \sigma(a_j) \). In supervised learning, the goal of NN training is to learn weights and bias terms in a NN function, which we denote by \( \hat{N}(x) \), given training data \((x_i, y_i)\) for \( 1 \leq i \leq n \), where \( x_i \in \mathbb{R}^d \) and \( y \in \mathbb{R} \). To introduce a continuous perspective, we assume that there is an underlying function \( g : \mathbb{R}^d \to \mathbb{R} \).
such that \( y_i = g(x_i) \) for \( 1 \leq i \leq n \) and the \( x_i \)'s are distributed according to a distribution \( \mu(x) \). The training procedure is often a gradient-based optimization algorithm that minimizes the residual in the squared \( L^2(d\mu) \) norm, i.e.,

\[
\Phi(W) = \frac{1}{2} \int |g(x) - \mathcal{N}(x; W)|^2 d\mu(x) \approx \frac{1}{2n} \sum_{i=1}^{n} |y_i - \mathcal{N}(x_i; W)|^2, 
\]

where \( W \) represents the weights and bias terms. In this paper, we consider ReLU NNs, which are NNs for which the activation function is the ReLU function given by \( \text{ReLU}(t) = \max(t, 0) \). The ReLU activation function has a useful multiplicative property that \( \text{ReLU}(\alpha t) = \alpha \text{ReLU}(t) \) for any \( \alpha > 0 \). Due to this property, we assume that the training samples are normalized so that \( x_1, \ldots, x_n \in S^{d-1} \).

Similar to most theoretical studies investigating frequency biasing, we restrict ourselves to 2-layer NNs [Arora et al. 2019, Basri et al. 2019, Su and Yang 2019, Cao et al. 2019]. To study NN training, it is common to consider the dynamics of \( \Phi(W) \) as one optimizes the weights and biases in \( W \). For example, the gradient flow of the NN weights is given by \( \frac{dW}{dt} = -\frac{\partial \Phi}{\partial W} \).

Define the residual \( z(x; W) = g(x) - \mathcal{N}(x; W) \). We have

\[
\frac{dz(x; W)}{dt} = -\int K(x, x'; W) z(x'; W) d\mu(x'), 
\]

where \( K(x, x'; W) = \left( \frac{\partial \mathcal{N}(x; W)}{\partial W}, \frac{\partial \mathcal{N}(x'; W)}{\partial W} \right) \). Under the assumptions that the weights do not change much during training, one can consider the NTK in the mean-field regime given the underlying time-independent distribution of \( W \), i.e., \( \mathcal{K}^\infty(x, x') = E_W[K(x, x'; W)] \) [Du et al. 2018]. Based on eq. (2), one can understand the decay of the residual by studying the reproducing kernel Hilbert space (RKHS) through a spectral decomposition of the integral operator \( \mathcal{L} \) defined by \( (\mathcal{L}z)(x) = \int \mathcal{K}^\infty(x, x') z(x') d\mu(x') \). Most results in the literature require \( \mu(x) \) to be the uniform distribution over the sphere so that the eigenfunctions of \( \mathcal{L} \) are spherical harmonics and the eigenvalues have explicit forms [Cao et al. 2019, Basri et al. 2019, Scetbon and Harchaoui 2021]. These explicit formulas for the eigenvalues and eigenfunctions of \( \mathcal{L} \) rely on the Funk–Hecke theorem, which provides a formula allowing one to express an integral over a hypersphere by an integral over an interval [Seeley 1966]. The frequency biasing of NN training can be explained by the fact that low-degree spherical harmonic polynomials are eigenfunctions of \( \mathcal{L} \) associated with large eigenvalues [Basri et al. 2019]. Thus, for uniform training data, the optimization of the weights and biases of an NN tends to fit the low-frequency components of the residual first.

When \( \mu(x) \) is nonuniform, it is difficult to analyze the spectral properties of \( \mathcal{L} \) and thus the frequency biasing properties of NN training. Since the Funk–Hecke formula no longer holds, there are only a few special cases where frequency biasing is understood [Williams and Rasmussen 2006, Sec. 4.3]. Although one may derive asymptotic bounds for the eigenvalues [Widom 1963, 1964, Bach and Jordan 2002], it is very hard to obtain formulas for the eigenfunctions, and one usually relies on numerical approximations [Baker 1977]. For the ReLU-based NTK, [Basri et al. 2020] provided explicit eigenfunctions assuming that the \( \mu(x) \) is piecewise constant on \( S^2 \), but this analysis does not generalize to higher dimension. To study the frequency biasing of NN training, one needs to understand both the eigenvalues and eigenfunctions of \( \mathcal{L} \), and this remains a significant challenge for a general \( \mu(x) \) due to the absence of the Funk–Hecke formula.

To overcome this challenge, we take a radically different point-of-view. While it is standard to discretize the integral in eq. (1) using a Monte Carlo-like average, we discretize it using a data-dependent quadrature rule where the nodes are at the training data. That is, we investigate frequency biasing of NN training when minimizing the residual in the standard squared \( L^2 \) norm:

\[
\tilde{\Phi}(W) = \frac{1}{2} \int |g(x) - \mathcal{N}(x; W)|^2 d\mu(x) \approx \frac{1}{2} \sum_{i=1}^{n} c_i |y_i - \mathcal{N}(x_i; W)|^2, 
\]

where \( c_1, \ldots, c_n \) are the quadrature weights associated with the (nonuniform) input data \( x_1, \ldots, x_n \). If \( x_1, \ldots, x_n \) are drawn from a uniform distribution over the hypersphere, then one can select \( c_i = A_d/n \) for \( 1 \leq i \leq n \), where \( A_d \) is the Lebesgue measure of the hypersphere; otherwise, one can choose any quadrature weights so that the integration rule is accurate (see section 4.2). If \( x_1, \ldots, x_n \) are drawn at random from \( \mu(x) \), then it is often reasonable to select \( c_i = 1/(np(x_i)) \), where \( d\mu(x) = p(x)dx \). While \( c_1, \ldots, c_n \) depend on \( x_1, \ldots, x_n \), the continuous expression for
\( \Phi(W) \) is always unaltered in eq. (3). Therefore, we can use the Funk–Hecke formula to analyze the eigenvalues and eigenfunctions of \( L \) defined by \( (Lz)(x) = \int K(x, x') z(x') dx' \), allowing us to understand frequency biasing.

In this paper, we propose to minimize the residual in a squared Sobolev \( H^s \) norm for a carefully selected \( s \in \mathbb{R} \). Unlike the \( L^2 \) norm (the case of \( s = 0 \)), the \( H^s \) norm for \( s \neq 0 \) has its own frequency bias. For \( s > 0 \), \( H^s \) penalizes high frequencies more than low, while for \( s < 0 \), low frequencies are penalized the most. We implement the squared \( H^s \) norm using a quadrature rule, which induces a different integral operator \( L_s \). We analyze the eigenvalues and eigenfunctions of \( L_s \), and consequently, the frequency biasing in the NN training using the Funk–Hecke formula. Given our new understanding of frequency biasing, we select \( s \) so that the \( H^s \) norm amplifies, dampens, counterbalances, or reverses the natural frequency biasing from an overparameterized NN training.

**Contributions.** We have three main contributions.

1. From our quadrature point-of-view, we analyze the frequency biasing in training a 2-layer overparameterized ReLU NN with nonuniform training data. In Theorem 2, we show that the theory of frequency biasing in [Basri et al. 2019] for uniform training data continues to hold in the nonuniform case up to quadrature errors. In Theorem 3, we provide control of the quadrature errors.

2. We use our knowledge of frequency biasing to modify the usual squared \( L^2 \) loss function to a squared \( H^s \) norm. By carefully selecting \( s \), we can amplify, dampen, counterbalance, or reverse the intrinsic frequency biasing in NN training and accelerate the observed convergence of gradient-based optimization procedures.

3. A potential issue with the \( H^s \) norm is the difficulties of implementing with high-dimensional training data. Using an image dataset of dimension \( 28^2 = 784 \), we show how to use an encoder-decoder architecture to implement a practical version of the squared \( H^s \) norm loss and adjust the frequency biasing in NN training to suppress noises of different frequencies. (see Figure 4).

2 Preliminaries and notation

For \( d > 1 \), let \( g : S^{d-1} \to \mathbb{R} \) be a square-integrable function defined on \( S^{d-1} \). The function \( g \) can be expressed in a spherical harmonic expansion given by

\[
 g(x) = \sum_{\ell=0}^{\infty} \sum_{p=1}^{N_d} \hat{g}_{\ell,p} Y_{\ell,p}(x), \quad \hat{g}_{\ell,p} = \int_{S^{d-1}} g(x) Y_{\ell,p}(x) dx,
\]

where \( Y_{\ell,p} \) is the spherical harmonic function of degree \( \ell \) and order \( p \). Here, \( N_d \) is the number of spherical harmonic functions of degree \( \ell \) so that \( N_d(0) = 1 \) and \( N_d(\ell) = (2\ell + d - 2)\Gamma(\ell + d - 2)/(\Gamma(\ell + 1)\Gamma(d - 1)) \) for \( \ell \geq 1 \). The set \( \{Y_{\ell,p}\}_{\ell \geq 0, 1 \leq p \leq N_d} \) is an orthonormal basis for \( L^2(S^{d-1}) \). Let \( H^d_{\ell} \) be the span of \( \{Y_{\ell,p}\}_{p=1}^{N_d(\ell)} \). Let \( H^d = \bigoplus_{\ell=0}^{\infty} H^d_{\ell} \) be the space of spherical harmonics of degree \( \leq \ell \).

Given distinct training data \( \{x_i\}_{i=1}^{m} \) from \( S^{d-1} \) and evaluations \( y_i = g(x_i) \) for \( 1 \leq i \leq n \), our goal is to understand the intrinsic frequency-biasing behavior of training a 2-layer ReLU NN given by

\[
 N(x) = \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \text{ReLU}(w_r^T x + b_r), \quad \text{ReLU}(t) = \max(t, 0),
\]

where \( m \) is the number of neurons, \( w_1, \ldots, w_m \) and \( a_1, \ldots, a_m \) are weights, and \( b_1, \ldots, b_m \) are the bias terms. We begin with the same setup as in [Basri et al. 2020]: assuming that (1) \( w_1, \ldots, w_m \) are initialized independently and identically distributed (iid) from Gaussian random variables with covariance matrix \( \kappa^2 I \), where \( \kappa > 0 \); (2) the bias terms are initialized to zero, and (3) \( a_1, \ldots, a_m \) are initialized iid as \( +1 \) with probability \( 1/2 \) and \( -1 \) otherwise, and \( \{a_r\} \) are not updated during the training process.

We use a gradient-based optimization scheme to train for the weights and biases and aim to minimize the residual defined by a symmetric positive definite matrix \( P \), which can be neatly written as

\[
 \Phi_P(W) = \frac{1}{2} (y - u)^T P (y - u),
\]
where \( y = (g(x_1), \ldots, g(x_n))^\top \) and \( u = (N(x_1), \ldots, N(x_n))^\top \). For example, we have \( P = n^{-1}I \) in eq. (1) and \( P = \text{diag}(c_1, \ldots, c_n) \) in eq. (3). Recall that \( W \) represents all the weights and biases of the NN. Given the loss function, we train the NN based on the gradient descent algorithm:

\[
w_r(k + 1) - w_r(k) = -\eta \frac{\partial \Phi_P}{\partial w_r}, \quad b_r(k + 1) - b_r(k) = -\eta \frac{\partial \Phi_P}{\partial b_r}.
\]

where \( k \) is the iteration number and \( \eta > 0 \) is the learning rate. The matrix \( P \) induces an inner product \( \langle \xi, \zeta \rangle_P = \xi^\top P \zeta \), which leads to a finite-dimensional Hilbert space with the norm \( \| \xi \|_P = \sqrt{\langle \xi, \xi \rangle_P} \). Given a matrix \( A \in \mathbb{R}^{n \times n} \), we define its operator norm \( \| A \|_P = \sup_{\xi \in \mathbb{R}^n, \| \xi \|_1 = 1} |A\xi|_P \).

Furthermore, we define the matrix \( H^\infty \in \mathbb{R}^{n \times n} \) by

\[
H^\infty_{ij} = \mathbb{E}_{\omega \sim N(0, \kappa^2 I)} \left[ \frac{\langle \omega^\top x_i + 1, \omega^\top y_j \rangle_\mathcal{L}}{2} \mathbb{I}_{\{\omega^\top x_i, \omega^\top y_j \geq 0\}} \right] = \frac{(\langle x_i^\top x_j + 1 \rangle - \arccos(\langle x_i^\top x_j \rangle))}{4\pi}.
\]

Note that due to the introduction of the biases, \( H^\infty \) is slightly different than the one in [Du et al. 2018, Arora et al. 2019]. In fact, in contrast with [Du et al. 2018], \( H^\infty \) defined in eq. (9) is positive definite regardless of the distribution of the training data, as shown in the supplementary material.

**Proposition 1.** If \( x_1, \ldots, x_n \) are distinct, then \( H^\infty \) in eq. (9) is symmetric and positive definite.

As a consequence of Proposition 1, the matrix \( H^\infty P \) has positive eigenvalues, which we denote by \( \lambda_{n-1} \geq \cdots \geq \lambda_0 > 0 \). One can view \( H^\infty \) as coming from sampling a continuous kernel \( K^\infty : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R} \) given by

\[
K^\infty(x, y) = K^\infty(\langle x, y \rangle) = \frac{(\langle x, y \rangle + 1)(\pi - \arccos(\langle x, y \rangle))}{4\pi},
\]

where \( \langle \cdot, \cdot \rangle \) is the \( \ell^2 \) inner-product. It is convenient to view \( H^\infty \) as being a discretization of \( K^\infty \) as the eigenvalues and eigenfunctions of \( K^\infty \) are known explicitly via the Funk–Hecke formula [Basri et al. 2019]. It follows that

\[
\int_{\mathbb{S}^{d-1}} K^\infty(x, y)Y_{\ell,p}(y')dy = \mu_\ell Y_{\ell,p}(x), \quad \ell \geq 0.
\]

The explicit formulas for \( \mu_\ell \) with \( \ell \geq 0 \) are given in the supplementary material. We find that \( \mu_\ell > 0 \) for all \( \ell \) and \( \mu_\ell \) is asymptotically \( O(\ell^{-d}) \) for large \( \ell \) [Basri et al. 2019, Bietti and Mairal 2019].

### 3 The convergence of neural network training with a general loss function

Given the NN model in eq. (5) and a general loss function \( \Phi_P \) in eq. (6), we are interested in the convergence rate of NN training. We study this by analyzing the convergence rate for each harmonic component. We start by presenting a convergence result that holds for any symmetric matrix \( P \) with positive eigenvalues.

**Theorem 1.** In eq. (5), suppose that \( w_1, \ldots, w_m \) are initialized iid from Gaussian random variables with covariance matrix \( \kappa^2 I \); \( b_1, \ldots, b_m \) are initialized to zero, and \( a_1, \ldots, a_m \) are initialized iid as +1 with probability \( 1/2 \) and −1 otherwise. Suppose the NN is trained with training data \( (x_i, y_i) \) for \( 1 \leq i \leq n \). loss function \( \Phi_P \) in eq. (6) for a symmetric positive definite matrix \( P \), and the training procedure is the gradient descent update rule eq. (7) with step size \( \eta \). Let \( \mathcal{N}_k \) be the NN function after the \( k \)-th iteration and \( u(k) = (N_k(x_1), \ldots, N_k(x_n)) \), where \( \mathcal{N}_0 \) is the initial NN function. Let an accuracy goal \( 0 < \epsilon < 1 \), a probability of failure \( 0 < \delta < 1 \), and a time span \( T > 0 \) be given. Then, there exist constants \( C_1, C_2 > 0 \) that depend only on the dimension \( d \) such that if \( 0 \leq \eta \leq 1/(2M_1 M_P n) \) (see eq. (9)), \( \kappa \leq C_1 \epsilon M_1^{-1} \sqrt{d/n} \), and \( m \) satisfies

\[
m \geq C_2 \frac{M_1^2 M_P^2 n^3}{\kappa^2 \epsilon^2} \left( \lambda_0^4 + \eta^4 T^4 \epsilon^4 \right) + \frac{M_1^4 M_P^4 n^2 \log(n/\delta)}{\epsilon^2} \left( \lambda_0^2 + \eta^2 T^2 \epsilon^2 \right),
\]

then with probability \( \geq 1 - \delta \), we have

\[
y - u(k) = (I - 2\eta H^\infty P)^k y + \epsilon(k), \quad \| \epsilon(k) \|_P \leq \epsilon, \quad 0 \leq k \leq T.
\]

Here, \( H^\infty \) is defined in eq. (9), \( y = (g(x_1), \ldots, g(x_n))^\top \), and \( \lambda_0 \) is the smallest eigenvalue of \( H^\infty \).
We defer the proof to the supplementary material, which uses techniques from [Su and Yang, 2019]. The main idea behind the proof is that $I - 2\eta H^\infty P$ is close to the transition matrix for the residual $y - u(k)$ when $m$ is large. By taking $k$ small, we can control the size of the initialization $u(0)$ and therefore obtain $y - u(k) \approx (I - 2\eta H^\infty P)^k (y - u(0)) \approx (I - 2\eta H^\infty P)^k y$. Furthermore, $M_1 M_\rho n$ is an upper bound on $\lambda_{n-1}$, i.e., the maximum eigenvalue of $H^\infty P$. Therefore, our rate of convergence does not vanish as the number of training data points $n \to \infty$, provided that $M_1 = O(n^{-1/2})$ and $M_\rho = O(n^{-1/2})$. This is the case when $P = n^{-1} I$, which corresponds to eq. (1).

So, we overcome the vanishing convergence rate issue that appears in previous analyses of frequency biasing [Arora et al., 2019; Basri et al., 2019].

4 Frequency biasing with an $L^2$-based loss function

The standard mean-squared loss function in eq. (I) corresponds to setting $c_i = 1/n$ for $1 \leq i \leq n$ in eq. (3). When $\mu$ is uniform, eq. (I) and eq. (3) are equivalent. When $\mu$ is nonuniform, we introduce a quadrature rule with nodes $x_1, \ldots, x_n$ and weights $c_1, \ldots, c_n$ to approximate the standard $L^2$ loss function eq. (3). The weights are selected so that for low-frequency functions $f : S^{d-1} \to \mathbb{R}$, the quadrature error

$$E_c(f) = \int_{S^{d-1}} f(x) dx - \sum_{i=1}^n c_i f(x_i)$$

(14)

is relatively small. A reasonable quadrature rule has positive weights for numerical stability and satisfies $\sum_{i=1}^n c_i = A_d$ so that it exactly integrates constants. The continuous squared $L^2$ loss function based on the Lebesgue measure is then discretized to be the square of a weighted discrete $\ell^2$ norm (see eq. (3)). Hence, we take $P = D_c = \text{diag}(c_1, \ldots, c_n)$, which is positive definite as the $c_i$’s are positive. For a vector $v \in \mathbb{R}^n$, we write $\|v\|^2_{c} = v^T D_c v$ and set $c_{\max} = \max_{1 \leq i \leq n} \{c_i\}$.

We now apply Theorem 1 to study the frequency biasing of NN training with the squared $L^2$ loss function eq. (3). We state these results in terms of quadrature errors. Recall our continuous setup where we assume that the training data is taken from a function $g : S^{d-1} \to \mathbb{R}$ so that $y_i = g(x_i)$ for $1 \leq i \leq n$. We further assume that $g$ is bandlimited with bandlimit $L$ where $g = g_0 + \cdots + g_L$ and $g_\ell \in H^\infty_{\ell}$ for $0 \leq \ell \leq L$. We define our quadrature errors as

$$c_{\ell,p}^n = E_c(g_j Y_{\ell,p}), \quad c_{\ell,p}^k = E_c(K^\infty(x_i, \cdot) Y_{\ell,p}), \quad c_{\ell,p}^e = E_c(g_j g_\ell), \quad c_{\ell,p}^{e,k} = E_c(K^\infty(x_i, \cdot) g_\ell),$$

(15)

where $1 \leq i \leq n, j, \ell \geq 0$, and $1 \leq p \leq N(d, \ell)$, and we interpret $g_\ell = 0$ when $\ell > L$.

4.1 A frequency-based formula for the training error

We obtain a similar result to [Arora et al., 2019, Thm. 4.1] when using the standard squared $L^2$ loss function eq. (3), except our step size does not depend on $\lambda_0$. Instead of expressing the training error in terms of the eigenvalues and eigenvectors of $H^\infty D_c$, we directly relate the training error to the frequency component of the target function $g$ and the eigenvalues of the continuous kernel $K^\infty$.

Theorem 2. Under the same setup and assumptions of Theorem 1, let $P = D_c$ and $M_1 = M_\rho = \sqrt{c_{\max}}$. If $g : S^{d-1} \to \mathbb{R}$ is a bandlimited function with bandlimit $L$ and $1 - 2\eta \mu_\ell > 0$ for all $0 \leq \ell \leq L$ (see eq. (1I)), then with probability $\geq 1 - \delta$ we have

$$\|y - u(k)\|_c = \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell)^2 \|g_\ell\|^2_{L^2} + \varepsilon_1(k) + \varepsilon_2 + \varepsilon_3(k), \quad |\varepsilon_3(k)| \leq \epsilon, \quad 0 \leq k \leq T,$$

(16)

where $\varepsilon_1(k)$ and $\varepsilon_2$ satisfy

$$|\varepsilon_1(k)| \leq \sum_{\ell=0}^{L} \sum_{j=\ell}^{L} (1 - 2\eta \mu_\ell)^k (1 - 2\eta \mu_\ell)^k \varepsilon_j^e \varepsilon_\ell^e, \quad |\varepsilon_2| \leq \sum_{\ell=0}^{L} \sqrt{A_{\ell}} \max_{1 \leq i \leq n} |\varepsilon_i^e|.$$

The proof of Theorem 2 is postponed to the supplementary material. Since $\sum_{i=1}^n c_i = A_d$, we expect that $c_i \to 0$ as $n \to \infty$. In fact, for most training data we expect that $c_{\max} = O(n^{-1})$ as $n \to \infty$. This means the step size $\eta$ does not decay as $n \to \infty$. Up to a quadrature error, $\|y - u(k)\|_c$ is close
to the standard $L^2$ norm of the residual function $g - N_k$. Explicit formulas for the eigenvalues $\{\mu_k\}$ (see eq. (11)) are given in [Basri et al. 2019], and it was shown that $\mu_k = O(2^{-d})$ [Bietti and Mairal 2019]. Theorem 2 demonstrates that the frequency biasing in NN training as the rate of convergence for frequency $0 \leq \ell \leq L$ is $1 - 2\mu_k$, which is close to 1 when $\ell$ is large. Therefore, we expect that NN training approximates the low-frequency content of $g$ faster than its high-frequency components. This is similar to the frequency biasing behavior derived for training with uniform data.

4.2 Estimating the quadrature errors

We now quantify the quadrature errors in Theorem 2. If we can design a quadrature rule at the training data $x_1, \ldots, x_n$ such that the quadrature error satisfies

$$|E_n(h)| = \left| \int_{g_{d-1}} h(x)dx - \sum_{i=1}^{n} c_i h(x_i) \right| \leq \gamma_{n,\ell} \|h\|_{L^\infty}, \quad h \in \Pi_d^\ell, \quad \ell \geq 0, \tag{17}$$

for some constant $\gamma_{n,\ell} \geq 0$, then we can bound the terms in eq. (15). We expect that for each fixed $\ell$, $\gamma_{n,\ell} \to 0$ as $n \to \infty$ as this is saying that integrals can be calculated more accurately for a large number of quadrature nodes. Under the reasonable assumption that our quadrature rule satisfies eq. (17), we can bound the quadrature errors appearing in Theorem 2.

Theorem 3. Under the same assumptions of Theorem 2 and that the quadrature rule satisfies eq. (17), there exist constants $C_1, C_2 > 0$ only depending on the dimension $d$ such that the terms $|\varepsilon_1(k)|$ and $|\varepsilon_2|$ in Theorem 2 satisfy

$$|\varepsilon_1(k)| \leq C_1 \left( \frac{L^3}{\ell} + L^2 \gamma_{n,\ell} \right) \max_{0 \leq j \leq L} \|g_j\|_{L^\infty}, \quad |\varepsilon_2| \leq C_2 \left( \frac{L^2}{\ell} + L \gamma_{n,\ell} \right) \max_{0 \leq j \leq L} \|g_j\|_{L^\infty} \sum_{j=0}^{L} \mu_j^{-1}$$

for all $k \geq 0, \ell \geq 1$, where $g = g_0 + \cdots + g_L$ with $g_j \in H_d^j$.

The proof is in the supplementary material. Theorem 3 states that $\varepsilon_1(k)$ and $\varepsilon_2$ can be made arbitrarily small if the quadrature errors converges to 0 as the number of nodes $n \to \infty$. In particular, if there is a sequence $\{\ell_n\}$ that increases to $\infty$ such that the quadrature rule is exact for all functions $h \in \Pi_d^{\ell_n}$, i.e., $E_n(h) = 0$, where $\ell_n \to \infty$ (see e.g. [Mhaskar et al. 2000], the rates of convergence of $\varepsilon_1(k)$ and $\varepsilon_2$ are both $O(1/\ell_n)$ for a fixed $g$. Without the quadrature being exact, we still have nice convergence provided the quadrature errors are small, as the following corollary shows.

Corollary 1. Suppose there exists a sequence $\ell_n \to \infty$ such that $\gamma_{n,\ell_n} \to 0$ as $n \to \infty$. Then, for a fixed $L \geq 0$, we have $\max_{k \geq 0, g \in \Pi_d^{\ell_n}} |\varepsilon_1(k)| / \|g\|_{L^2}^2$ and $\max_{g \in \Pi_d^{\ell_n}} |\varepsilon_2| / \|g\|_{L^2} \to 0$ as $n \to \infty$.

Corollary 1 shows that as $n$ increases, the quadrature errors $\varepsilon_1(k)$ and $\varepsilon_2$ converge to zero. Moreover, this convergence is uniform in the sense that it does not depend on the specific choice of $g \in \Pi_d^\ell$. Here, we normalize $\varepsilon_1(k)$ and $\varepsilon_2$ by $\|g\|_{L^2}^2$ and $\|g\|_{L^2}$, respectively, to obtain the “relative” quadrature errors that do not scale when $g$ is multiplied by a scalar (see (16)).

5 Frequency biasing with a Sobolev-norm loss function

The frequency biasing during the training of an overparameterized NN has several consequences. In some situations, worse convergence rates for high-frequency components of a function are beneficial since the NN training procedure is less sensitive to the oscillatory noise in the data, acting as a low-pass filter. This significantly improves the generalization error of overparameterized NNs. However, in other situations, NN training struggles to accurately learn the high-frequency content of $g$, resulting in slow convergence. To precisely control the frequency biasing of NN training, we propose to train a NN with a loss function that has intrinsic spectral bias. One such example is the so-called Sobolev norm. Given $s \in \mathbb{R}$, the spherical Sobolev space is defined as

$$H^s(\mathbb{S}^{d-1}) = \left\{ f \in L^2(\mathbb{S}^{d-1}) \left| \|f\|_{H^s(\mathbb{S}^{d-1})}^2 = \sum_{\ell=0}^{\infty} \sum_{p=1}^{N(d,\ell)} (1 + \ell)^{2s} |\hat{f}_{\ell,p}|^2 < \infty \right. \right\},$$

where $\hat{f}_{\ell,p}$ are the spherical harmonic coefficients of $f$ (see eq. (4)) and $N(d,\ell)$ is given in Section 2. We propose to set the loss function to be $\frac{1}{2} \|g - N\|_{H^s}^2$ in replace of $\frac{1}{2} \|g - N\|_{L^2}^2$ in eq. (3). When
s = 0, the $H^0$ Sobolev norm reduces to the $L^2$ norm as all spherical harmonic coefficients have an equal weight of 1. If $s > 0$, then the high-frequency spherical harmonic coefficients are amplified by $(1 + \ell)^{2s}$. The high-frequency components of the residual are then penalized more in the loss function. Hence, we expect the NN training to learn the high-frequency components faster with the squared $H^s$ loss function than the case of eq. (3). Similarly, if $s < 0$, then the high-frequency spherical harmonic coefficients are dampened by $(1 + \ell)^{2s}$. Consequently, one expects that the NN training process captures the high-frequency components of the residual more slowly with the squared $H^s$ loss function. However, when $s < 0$, we expect that the training is more robust to high-frequency noise in the training data. By tuning the parameter $s$, we can control the frequency biasing in NN training (see Theorem 4). The choice of $s$ for a particular application can be determined from theory or by cross-validation.

First, we justify that the residual function is indeed in $H^s$. Since we assume that $g$ is bandlimited, $g \in H^s$ for all $s \in \mathbb{R}$. Proposition 2 shows that we could consider $s < 3/2$ for ReLU-based NN.

**Proposition 2.** Suppose $\mathcal{N} : \mathbb{S}^{d-1} \to \mathbb{R}$ is a 2-layer ReLU NN (see eq. (5)). Then, we have $\mathcal{N} \in H^s(\mathbb{S}^{d-1})$ for all $s < 3/2$. Moreover, if $s \geq 3/2$, $\mathcal{N} \in H^s(\mathbb{S}^{d-1})$ if and only if $\mathcal{N}$ is affine.

The proof is deferred to the supplementary material. When $s \geq 3/2$, the residual function $\mathcal{N} - g$ may not be in $H^s$. However, we can still use the truncated sum to a maximum frequency $\ell_{\text{max}}$ to train the NN, although the sum can no longer be interpreted as an approximation of some Sobolev norm at the continuous level. We discretize the Sobolev-based loss function as

$$\Phi_s(W) = \frac{1}{2} \sum_{\ell=0}^{\ell_{\text{max}}} \sum_{p=1}^{N(d, \ell)} (1 + \ell)^{2s} c_i Y_{\ell,p}(x_i)(g - \mathcal{N})(x_i) \geq \frac{1}{2} (y - u)^\top P_s (y - u), \quad (18)$$

where $u$ and $y$ follow eq. (9), and $P_s = \sum_{\ell=0}^{\ell_{\text{max}}} \sum_{p=1}^{N(d, \ell)} (1 + \ell)^{2s} P_{\ell,p}, P_{\ell,p} = \mathbf{a}_s x_e^\top, \text{and } (\mathbf{a}_s)_{ij} = c_i Y_{\ell,p}(x_i)$. We assume that $P_s$ is positive definite, which requires that $(\ell_{\text{max}} + 1)^2  \geq n$. Next, we present our convergence theorem for Sobolev training.

**Theorem 4.** Suppose $g \in \Pi_L^d$ and $\Phi_s$ is the loss function in eq. (13), where $P_s$ is positive definite and $\ell_{\text{max}} \geq L$. Under the assumptions of Theorem 1 if $1 - 2\eta \mu_{\ell}(1 + \ell)^{2s} > 0$ for all $0 \leq \ell \leq L$, then with probability $\geq 1 - \delta$ over the random initialization, we have

$$u(k) - y = \sum_{\ell=0}^{L} (1 - 2\eta \mu_{\ell}(1 + \ell)^{2s})^k y^{\ell} + \varepsilon_1 + \varepsilon_2(k), \quad \|\varepsilon_2(k)\|_{P_s} \leq \epsilon, \quad 0 \leq k \leq T,$$

where $y^{\ell} = (g_\ell(x_1), \ldots, g_\ell(x_n))^\top$ and $\varepsilon_1$ satisfies

$$\|\varepsilon_1\|_{P_s} \leq \sum_{\ell=0}^{L} \mu_{\ell}^{-1} \|\varepsilon_1^{(\ell)}\|_{P_s}, \quad (\varepsilon_1^{(\ell)})_i = e_{i,0}^{(\ell)} + \sum_{j=0}^{\ell_{\text{max}}} \sum_{p=1}^{N(d, j)} e_{i,j,p}^{(\ell)} \mu_{j} Y_{\ell,p}(x_i) + e_{i,j,p}^{(\ell)},$$

Compared to Theorem 2, Theorem 4 says that up to the level of quadrature errors, the convergence rate of the degree-$\ell$ component is $1 - 2\eta \mu_{\ell}(1 + \ell)^{2s}$. In particular, since $\mu_{\ell} = \mathcal{O}(\ell^{-d})$, there is a $s^* > 0$, which depends on $d$, such that $(1 + \ell)^{2s^*} \mu_{\ell}$ can be bounded from above and below by positive constant that are independent of $\ell$ for all $\ell \geq 0$. This means for any $s > s^*$, we expect to reverse the frequency biasing behavior of NN training. Figure 2 shows the reversal of frequency biasing as $s$ increases from $-1$ to $4$ (see section 6.1).

## 6 Experiments and discussion

This section presents three experiments with synthetic and real-world datasets to investigate the frequency biasing of NN training using squared $L^2$ loss and squared $H^s$ loss. The first two experiments learn functions on $\mathbb{S}^1$ and $\mathbb{S}^2$, respectively. In the third test, we train an autoencoder on the MNIST dataset for a denoising task. One can find more details in the supplementary material.

### 6.1 Learning trigonometric polynomials on the unit circle

First, we consider learning a function on $\mathbb{S}^1$. We create a set of $n = 1140$ nonuniform data $\{x_i\}_{i=1}^n$, as seen in Figure 1 and compute the quadrature weights $\{c_i\}_{i=1}^n$ for the loss function $\Phi$ in eq. (5).
We also use the squared $H^s$ loss function. We train a 2-layer ReLU NN to learn $g(x) = \tilde{g}(\theta) = \sum_{\ell=1}^s \sin(\ell \theta)$, where $x = (\cos \theta, \sin \theta)$. We define the frequency loss $|\hat{N}(\ell) - \hat{g}(\ell)|$ as the loss function $\Phi$ in eq. (1) and $\tilde{\Phi}$ in eq. (3), respectively. The comparison shows that the frequency biasing is more evident given the loss function $\Phi$. This observation collaborates the theoretical statements in Theorem 2. There is no guarantee that frequency biasing always exists when using $\Phi$ as the loss function for nonuniform data training, which is also observed here. Moreover, Figure 1 also shows that it takes asymptotically $O(\ell^2)$ iterations to learn the $\ell$th frequency $\sin(\ell \theta)$ given the loss function $\tilde{\Phi}$. A similar plot appears in Basri et al. [2019] for uniform data training.

We also use the squared $H^s$ norm as the loss function to learn $g$. After 5000 epochs, we plot the $\ell$th frequency loss with $\ell$ ranging from 1 (blue) to 9 (red) in Figure 2, given different $s$ values. As $s$ increases, the higher-frequency components are learned faster. When $s > 2$, the frequency biasing is entirely reversed in the sense that higher-frequency parts are learned faster than the lower-frequency ones rather than a low-frequency biasing under the squared $L^2$ loss (see Theorem 2). The gradually changing “rainbow” in Figure 2 demonstrates that the smoothing property of an overparameterized NN can be compensated by the intrinsic high-frequency biasing of the $H^s$ loss function for a large enough $s$, corroborating Theorem 4.

6.2 Learning spherical harmonics on the unit sphere

Similar to the previous example in $S^1$, we design an experiment on $S^2$. We utilize a data set $\{x_i\}_{i=1}^n$ in Wright and Michaels [2015] where $n = 2500$, which comes with carefully designed positive
Figure 3: Frequency losses for $\ell = 4$ (blue), 10 (red), and 20 (yellow), when learning a function on $\mathbb{S}^2$ using different squared $H^s$ loss function. Compared to low-frequency biasing in the cases of $s = -1$ (left) and $s = 0$ (middle), we observe a high-frequency biasing when $s = 2.5$ (right).

Figure 4: The output of a squared $H^s$ loss-trained autoencoder on a typical test image when the input images are contaminated by low-frequency noise (top row) and high-frequency noise (bottom row).

quadrature weights $\{c_i\}_{i=1}^n$. We test the squared $H^s$ norm as the loss function in NN training with training data coming from a function $g(x) = \sum_{\ell=0, \ell \text{ even}}^{30} Y_{\ell,0}$ defined on $\mathbb{S}^2$ that involves more high-frequency components than the $\mathbb{S}^1$ example. The training results are shown in Figure 3 with different $s$ values. The natural low-frequency biasing of NN in the case of $L^2$-based training (the case of $s = 0$) is enhanced when $s = -1$, and is totally reversed when $s = 2.5$.

6.3 Autoencoder on the MNIST dataset

The idea of Sobolev training is also useful for high-dimensional training data. Here, we present the results of the autoencoder for image denoising using the MNIST dataset [LeCun et al. 2010]. In Figure 4, the outputs of the autoencoder are presented when trained with the squared $H^s$ norm as the loss function. We contaminate the dataset with random low-frequency noise (top row) and high-frequency noise (bottom row). When high-frequency noise is present, the $H^s$ loss function generally performs better with $s < 0$, while the case of $s > 0$ helps image deblurring when the input image suffers from low-frequency noise. This corroborates our discussion in Section 5.

7 Conclusions

We observe a frequency biasing in NN training even with nonuniform training data. Instead of the standard mean-squared loss function in eq. (1), we propose the use of a different loss function in eq. (3), which involves quadrature weights and has a natural continuous analogue. With eq. (3), we prove that frequency biasing always exists with nonuniform data and rigorously analyze it using the Funk–Hecke formula. While the frequency biasing phenomena of NN training improves its generalization error, it also makes it difficult to learn highly oscillatory components of a function. By changing the loss function to a squared Sobolev-based loss function, we can control the frequency biasing in NN training, which can accelerate NN training convergence and improve stability.
References

S. Arora, S. S. Du, W. Hu, Z. Li, and R. Wang. Fine-grained analysis of optimization and generalization for overparameterized two-layer neural networks. In Inter. Conf. Mach. Learn., pages 322–332. PMLR, 2019.

F. R. Bach and M. I. Jordan. Kernel independent component analysis. J. Mach. Learn. Res., 3(Jul):1–48, 2002.

C. T. H. Baker. The numerical treatment of integral equations. Oxford University Press, 1977.

J. A. Barceló, T. Luque, and S. Pérez-Esteva. Characterization of Sobolev spaces on the sphere. J. Math. Anal. Appl., 491(1):124240, 2020.

R. Basri, D. Jacobs, Y. Kasten, and S. Kritchman. The convergence rate of neural networks for learned functions of different frequencies. Adv. Neur. Info. Proc. Syst., 32, 2019.

R. Basri, M. Galun, A. Geifman, D. Jacobs, Y. Kasten, and S. Kritchman. Frequency bias in neural networks for input of non-uniform density. In Inter. Conf. Mach. Learn., pages 685–694. PMLR, 2020.

M. Belkin, D. Hsu, S. Ma, and S. Mandal. Reconciling modern machine-learning practice and the classical bias–variance trade-off. Proc. Nat. Acad. Sci., 116(32):15849–15854, 2019.

A. Bietti and J. Mairal. On the inductive bias of neural tangent kernels. Adv. Neur. Info. Proc. Syst., 32, 2019.

Y. Cao, Z. Fang, Y. Wu, D.-X. Zhou, and Q. Gu. Towards understanding the spectral bias of deep learning. arXiv preprint arXiv:1912.01198, 2019.

F. Chollet. Building autoencoders in keras. https://blog.keras.io/building-autoencoders-in-keras.html, 2016.

F. Dai and Y. Xu. Approximation theory and harmonic analysis on spheres and balls, volume 23. Springer, 2013.

S. S. Du, X. Zhai, B. Poczos, and A. Singh. Gradient descent provably optimizes over-parameterized neural networks. Inter. Confer. Learn. Rep., 2018.

B. Engquist, K. Ren, and Y. Yang. The quadratic Wasserstein metric for inverse data matching. Inverse Problems, 36(5):055001, 2020.

S. Fridovich-Keil, R. Gontijo-Lopes, and R. Roelofs. Spectral bias in practice: The role of function frequency in generalization. arXiv preprint arXiv:2110.02424, 2021.

W. Hoeffding. Probability inequalities for sums of bounded random variables. J. Amer. Stat. Assoc., 58:13–30, 1963.

A. Jacot, F. Gabriel, and C. Hongler. Neural tangent kernel: Convergence and generalization in neural networks. Adv. Neur. Info. Proc. Syst., 31, 2018.

Y. LeCun, C. Cortes, and C. J. Burges. MNIST handwritten digit database. ATT Labs [Online]. Available: http://yann.lecun.com/exdb/mnist, 2, 2010.

S. Li. Concise formulas for the area and volume of a hyperspherical cap. Asian J. Math. Stat., 4:66–70, 2011.

D. Lozier et al. Nist digital library of mathematical functions. (38), 2003-05-01 2003. URL https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=150849

H. N. Mhaskar, F. J. Narcowich, and J. D. Ward. Spherical Marcinkiewicz–Zygmund inequalities and positive quadrature. Math. Comp., 70(235):1113–1130, 2000.

N. Rahaman, A. Baratin, D. Arpit, F. Draxler, M. Lin, F. Hamprecht, Y. Bengio, and A. Courville. On the spectral bias of neural networks. In Inter. Conf. Mach. Learn., pages 5301–5310. PMLR, 2019.

M. Scetbon and Z. Harchaoui. A spectral analysis of dot-product kernels. In Inter. Conf. Art. Intell. and Stat., pages 3394–3402. PMLR, 2021.

R. T. Seeley. Spherical harmonics. Amer. Math. Mon., 73(4P2):115–121, 1966.

L. Su and P. Yang. On learning over-parameterized neural networks: A functional approximation perspective. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, Adv. Neur. Info. Proc. Syst., volume 32. Curran Associates, Inc., 2019.
We train with the loss function given in eq. (6) so that the gradient descent algorithm for NN training is given by eq. (7). An important object in understanding the frequency biasing of NN training is the symmetric and positive definite matrix $H^\infty \in \mathbb{R}^{n \times n}$ in eq. (9). Since $H^\infty$ are symmetric positive definite matrices (see Proposition 1), $H^\infty P$ has positive real eigenvalues. To see this, note that $H^\infty P = H^\infty P^{1/2} P^{1/2} = P^{-1/2} (H^\infty P^{1/2}) P^{1/2}$. This means that $H^\infty P$ and $P^{1/2} H^\infty P^{1/2}$ are similar. Since the matrix $P^{1/2} H^\infty P^{1/2}$ is symmetric positive definite, $H^\infty P$ has positive eigenvalues. We denote the eigenvalues of $H^\infty P$ by $\lambda_{n-1} \geq \cdots \geq \lambda_0 > 0$, which partially govern the frequency biasing phenomena.

It is convenient to analyze the eigenvalues and eigenvectors of $H^\infty P$ via the zonal kernel $K^\infty : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \rightarrow \mathbb{R}$ given in eq. (10). The key is the Funk–Hecke formula [Seeley, 1966].

**Theorem 5** (Funk–Hecke). Suppose $K : [-1, 1] \rightarrow \mathbb{R}$ is measurable and $K(t) (1 - t^2)^{(d-3)/2}$ is integrable on $[-1, 1]$. Then, for any $h \in \mathcal{H}_d$, we have

$$
\int_{\mathbb{S}^{d-1}} K((\xi, \zeta)) h(\xi) d\xi = \left( A_d \int_{-1}^1 K(t) P_{\ell,d}(t)(1 - t^2)^{(d-3)/2} dt \right) h(\zeta), \quad \zeta \in \mathbb{S}^{d-1},
$$

(19)

where $P_{\ell,d}$ is the ultraspherical polynomial given by

$$
P_{\ell,d}(t) = \frac{(-1)^\ell \Gamma((d-1)/2)}{2^{\ell} \Gamma(\ell + (d-1)/2)(1 - t^2)^{(d-3)/2}} d\ell (1 - t^2)^{\ell+(d-3)/2}.
$$

(20)

Applying Theorem 5 we have that

$$
\int_{\mathbb{S}^{d-1}} K^\infty(x, y) h(y) d\sigma(y) = \mu_\ell h(x), \quad h \in \mathcal{H}_d,
$$

where $\mu_\ell > 0$, $\forall \ell$, given by [Basri et al., 2019].

$$
\mu_\ell = \begin{cases}
\frac{1}{2} C_1^d(0) \left( \frac{(d-1)/2}{p} \right) + \frac{2^{d-2}}{(d-1)(d+1)/2} - \frac{1}{2} \sum_{p+1=0}^{d-3} (-1)^p \left( \frac{d-3}{p} \right) \frac{1}{2p+1} , & \ell = 0,
\frac{1}{2} C_1^d(1) \sum_{p=\frac{d+3}{2}}^{\ell} \left( C_2^d(p, 1) \left( \frac{1}{2(2p+1)} \right) + \frac{1}{2p} \left( 1 - \frac{1}{2p} \left( \frac{2p}{d} \right) \right) \right) , & \ell = 1,
\frac{1}{2} C_1^d(\ell) \sum_{p=\frac{d+3}{2}}^{\ell} C_2^d(p, \ell) \left( \frac{1}{2(2p+2)} \right) \left( 1 - \frac{1}{2p} \left( \frac{2p}{d} \right) \right) , & \ell \geq 2 \text{ even},
\frac{1}{2} C_1^d(\ell) \sum_{p=\frac{d+3}{2}}^{\ell} C_2^d(p, \ell) \left( \frac{1}{2p} \left( \frac{2p-\ell+1}{d} \right) \right) , & \ell \geq 2 \text{ odd},
\end{cases}
$$

for $d \geq 3$, $d$ odd, where

$$
C_1^d(\ell) = \frac{(-1)^\ell 2^{p(d-1)/2}}{(d-1)2^\ell \Gamma(\ell + (d-1)/2)}, \quad C_2^d(p, \ell) = (-1)^p \left( \frac{\ell + d-3}{p} \right) \frac{(2p)!}{(2p-\ell)!}.
$$
Here, the exclamation mark means a factorial and \((\cdot)\) denotes the binomial coefficient.

Given \(\mathbf{x}, \mathbf{w}_r,\) and \(b_t\) in eq. 5, we write \(\bar{\mathbf{x}} = \frac{1}{\sqrt{2}}(\mathbf{x}, 1) \in \mathbb{S}^d\) and \(\bar{\mathbf{w}}_r = (\mathbf{w}_r, b_r) \in \mathbb{R}^{d+1}\). Therefore, we have \(\text{ReLU}(\mathbf{w}_r^T \mathbf{x} + b_r) = \sqrt{2} \text{ReLU}(\bar{\mathbf{w}}_r^T \bar{\mathbf{x}})\) and the NN function can be rewritten as

\[
\mathcal{N}(\mathbf{x}) = \frac{\sqrt{2}}{\sqrt{m}} \sum_{r=1}^m a_r \text{ReLU}(\bar{\mathbf{w}}_r^T \bar{\mathbf{x}}).
\]

By replacing the expectation over random initialization of \(\bar{\mathbf{w}}\) by \(\bar{\mathbf{w}}(t)\), we define the instantiations of \(\mathcal{H}^{\infty}\) at the \(k\)th iteration by \(\mathcal{H}(k)\), where

\[
H_{ij}(k) = \frac{1}{m} \bar{x}_i^T \bar{x}_j \sum_{r=1}^m \mathbb{I}\{\bar{x}_r^T \bar{\mathbf{w}}_r(k) \geq 0, \bar{x}_r^T \bar{\mathbf{w}}_r(k) \geq 0\},
\]

where \(\mathbb{I}\) is an indicator function.

**B The matrix \(\mathcal{H}^{\infty}\) is symmetric and positive definite**

Proposition 1 states that the matrix \(\mathcal{H}^{\infty}\) defined by eq. 9 is symmetric and positive definite. While the symmetry of \(\mathcal{H}^{\infty}\) is immediate from its closed-form expression, the fact that it is positive definite requires a more detailed analysis. The proof idea is similar to that of Theorem 3.1 of Du et al. [2018], in which the matrix \(\mathcal{H}^{\infty}\) is associated with a 2-layer ReLU NN without biases. However, our \(\mathcal{H}^{\infty}\) is associated with a 2-layer ReLU NN with biases. While Du et al. [2018] requires no two training data points are parallel, we allow the existence of \(x_{i_1} = -x_{i_2}\) for some \(i_1\) and \(i_2\). Hence, our proof employs on a pair of nodes denoted by \(x_{i_1}, x_{i_2}\).

**Proof of Proposition 1** For a measurable function \(f : \mathbb{R}^d \to \mathbb{R}^{d+1}\), we define a norm of \(f\) as

\[
\|f\|^2_{\mathcal{H}} = \mathbb{E}_{\mathbf{w} \sim \mathcal{N}(0, \kappa^2 \mathbf{I})} \|f(\mathbf{w})\|^2_{2},
\]

and let \(\mathcal{H}\) be the space of measurable functions such that \(\|f\|_{\mathcal{H}} < \infty\). It can be shown that \(\mathcal{H}\) is a Hilbert space with respect to the inner product \((f, g)_{\mathcal{H}} = \mathbb{E}_{\mathbf{w} \sim \mathcal{N}(0, \kappa^2 \mathbf{I})} \left[ f(\mathbf{w})^T g(\mathbf{w}) \right]\). For each \(x_i, 1 \leq i \leq n\), we define the function \(\phi_i\) by

\[
\phi_i(\mathbf{w}) = \bar{x}_i \mathbb{I}\{\mathbf{w}^T \bar{x}_i \geq 0\}, \quad \mathbf{w} \in \mathbb{R}^d. \tag{21}
\]

Then, \(\phi_i \in \mathcal{H}\) for all \(i\), and \(H_{ij}^\infty = \langle \phi_i, \phi_j \rangle_{\mathcal{H}}\). We prove that \(\mathcal{H}^{\infty}\) is positive definite by showing that \(\{\phi_i\}_{i=1}^n\) is a linearly independent set in \(\mathcal{H}\).

To show \(\{\phi_i\}_{i=1}^n\) is a linearly independent set, we show that

\[
\alpha_1 \phi_1(\mathbf{w}) + \cdots + \alpha_n \phi_n(\mathbf{w}) = 0 \quad \text{for almost every } \mathbf{w} \in \mathbb{R}^d \tag{22}
\]

implies that \(\alpha_i = 0\) for \(1 \leq i \leq n\). We fix some \(1 \leq i_1 \leq n\) and, without loss of generality, assume that \(x_{i_1} = -x_{i_2}\). Define the set \(D_j = \{\mathbf{w} \in \mathbb{R}^d \mid \mathbf{w}^T x_j = 0\}\) for \(1 \leq j \leq n\). As a result, \(D_1 = D_{i_2}\). Since each \(D_j\) is a hyperplane passing through the origin and \(D_i \neq D_j\) for any \(j \neq i_1, i_2, \exists \mathbf{z} \in D_i\) such that \(\mathbf{z} \notin D_j\) for any \(j \neq i_1, i_2\). For a positive radius \(R > 0\), let \(B_R = B(\mathbf{z}, R)\) be the ball centered at \(\mathbf{z}\) of radius \(R\). Define a partition of \(B_R\) into two sets denoted by \(B_R^+\) and \(B_R^-\) (possibly missing a subset of \(B_R\) that has zero Lebesgue measure), where

\[
B_R^+ = \{\mathbf{w} \in B_R \mid \mathbf{w}^T x_{i_1} > 0\} = \{\mathbf{w} \in B_R \mid \mathbf{w}^T x_{i_2} < 0\},
\]

\[
B_R^- = \{\mathbf{w} \in B_R \mid \mathbf{w}^T x_{i_1} < 0\} = \{\mathbf{w} \in B_R \mid \mathbf{w}^T x_{i_2} > 0\}.
\]

Since \(D_j\) is closed for each \(1 \leq j \leq n\), \(B_R\) is eventually disjoint from \(D_j\) as \(R \to 0\). Hence, we have

\[
\lim_{R \to 0} \sup_{\mathbf{w} \in B_R} |\phi_j(\mathbf{z}) - \phi_j(\mathbf{w})| = 0, \quad j \neq i_1, i_2, \tag{23}
\]

1 Otherwise, if such \(i_2\) does not exist, we can add an element \(\phi_{n+1}\) associated with \(-x_{i_1}\) to \(\{\phi_i\}_{i=1}^n\). If we can show \(\{\phi_i\}_{i=1}^{n+1}\) is linearly independent, then so is \(\{\phi_i\}_{i=1}^n\).
where $|\cdot|$ denotes the Euclidean distance. Then, for any $j \neq i_1, i_2$, we have
\[
\lim_{R \to 0} \frac{1}{|B^+_R|} \int_{B^+_R} \phi_j(w) dw = \phi_j(z), \quad \lim_{R \to 0} \frac{1}{|B^-_R|} \int_{B^-_R} \phi_j(w) dw = \phi_j(z).
\]
Consequently, we find that
\[
\lim_{R \to 0} \left( \frac{1}{|B^+_R|} \int_{B^+_R} \phi_j(w) dw - \frac{1}{|B^-_R|} \int_{B^-_R} \phi_j(w) dw \right) = 0, \quad j \neq i_1, i_2.
\]
Now, consider the integral of $\phi_{i_1}$ and $\phi_{i_2}$. We have
\[
\lim_{R \to 0} \left( \frac{1}{|B^+_R|} \int_{B^+_R} \phi_{i_1}(w) dw - \frac{1}{|B^-_R|} \int_{B^-_R} \phi_{i_1}(w) dw \right) = \lim_{R \to 0} \left( \frac{1}{|B^+_R|} \int_{B^+_R} \phi_{i_2}(w) dw - \frac{1}{|B^-_R|} \int_{B^-_R} \phi_{i_2}(w) dw \right) = \hat{x}_{i_1},
\]
\[
\lim_{R \to 0} \left( \frac{1}{|B^+_R|} \int_{B^+_R} \phi_{i_2}(w) dw - \frac{1}{|B^-_R|} \int_{B^-_R} \phi_{i_2}(w) dw \right) = \lim_{R \to 0} \left( \frac{1}{|B^+_R|} \int_{B^+_R} 0 dw - \frac{1}{|B^-_R|} \int_{B^-_R} \phi_{i_2}(w) dw \right) = -\hat{x}_{i_2}.
\]
By applying these limiting expressions to $\sum_{j=1}^n \alpha_j \phi_j(w) = 0$, we find that $\alpha_{i_1} \hat{x}_{i_1} - \alpha_{i_2} \hat{x}_{i_2} = 0$.
Since the last entries of both $\hat{x}_{i_1}$ and $\hat{x}_{i_2}$ are $1/\sqrt{2}$, we have $\alpha_{i_1} = \alpha_{i_2}$. Thus, we have $\alpha_{i_1} = 0$ because $x_{i_1} \neq 0$. Since $i_1$ is arbitrary, the statement of the proposition follows.

C The convergence of neural network training

In this section, we develop the theory for learning a NN with a general loss function $\Phi_P$ defined by a positive definite matrix $P$ in eq. (6). In particular, we prove Theorem [1] which states that the learning rate is sufficiently small, the weights are initialized without too much variance, and the NN is sufficiently wide, then the residual in the first few epochs can be described with the matrix $H^+P$.

While our proof is similar to that of Su and Yang [2019], the argument is distinct in three essential ways: (1) Our proof applies to any loss function defined by a positive definite matrix $P$, which requires us to use a different Hilbert space $\mathbb{R}_n$, $(\cdot, \cdot)_P$. (2) While the result in Su and Yang [2019] bounds the residual using the minimum eigenvalue of $H^\infty$, we estimate the residual as a matrix-vector product of $(I - 2\eta H^\infty P)^k y$, which allows us to analyze the training error using all eigenvalues of $H^\infty P$. (3) We use a different NN function that incorporates the bias terms and we do not assume that we initialize the weights in a way that makes $\mathcal{N}_0 = 0$.

Before we prove the theorem, we define some useful quantities. Let $A$ be the set of indices such that the coefficients $a_r$ are initialized to 1 and let $B$ be the set initialized to $-1$. We then decompose $H(k)$ into two parts, where $H(k)$ is defined in eq. (21), so that $H(k) = H^+(k) + H^-(k)$ with
\[
H^+_{ij}(k) = \frac{1}{m} \hat{x}_i^T \hat{x}_j \sum_{r \in A} \mathbb{I} \{ \hat{w}_r(k)^T \hat{x}_r \geq 0 \}, \quad H^-_{ij}(k) = \frac{1}{m} \hat{x}_i^T \hat{x}_j \sum_{r \in B} \mathbb{I} \{ \hat{w}_r(k)^T \hat{x}_r \geq 0 \}.
\]
Similarly, we define two other matrices $\tilde{H}^+(k)$ and $\tilde{H}^-(k)$ as
\[
\tilde{H}^+_{ij}(k) = \frac{1}{m} \hat{x}_i^T \hat{x}_j \sum_{r \in A} \mathbb{I} \{ \hat{w}_r(k+1)^T \hat{x}_r \geq 0 \}, \quad \tilde{H}^-_{ij}(k) = \frac{1}{m} \hat{x}_i^T \hat{x}_j \sum_{r \in B} \mathbb{I} \{ \hat{w}_r(k+1)^T \hat{x}_r \geq 0 \}.
\]
Unfortunately, $\tilde{H}^+(k)$ and $\tilde{H}^-(k)$ are not necessarily symmetric and they differ from $H^+(k)$ and $H^-(k)$ up to sign flips. To simplify the notation later, we also define two auxiliary matrices $L(k)$ and $M(k)$ as
\[
L(k) = \tilde{H}^+(k) - H^+(k), \quad M(k) = \tilde{H}^-(k) - H^-(k).
\]
We now prove that $I - 2\eta H(k)$ is close to the transition matrix for the residual, up to sign flips, i.e., $y - u(k+1) \approx (I - 2\eta H(k)) (y - u(k))$.

Lemma 1. Let $z(k) = y - u(k)$ be the residual after the $k$th iteration. For any $k \geq 0$ and $\eta > 0$, we have
\[
\left( I - 2\eta \left( \tilde{H}^+(k) + \tilde{H}^-(k) \right) P \right) z(k) \leq z(k+1) \leq \left( I - 2\eta \left( H^+(k) + H^-(k) \right) P \right) z(k),
\]
where the inequalities are entry-wise.
Proof. First, by the gradient descent update rule, we have
\[
\dot{\mathbf{w}}_r(k+1) - \dot{\mathbf{w}}_r(k) = -\eta \frac{\partial \Phi \mathbf{P}(\mathbf{w}_1(k), \ldots, \mathbf{w}_m(k))}{\partial \mathbf{w}_r} = -\eta \frac{\partial \mathbf{u}(k)}{\partial \mathbf{w}_r} \frac{\partial \Phi \mathbf{P}(\mathbf{u})}{\partial \mathbf{u}},
\]
where the \((d+1) \times n\) Jacobian matrix is given by
\[
\frac{\partial \mathbf{u}(k)}{\partial \mathbf{w}_r} = \sqrt{2\eta} \frac{\mathbf{a}_r}{\sqrt{m}} \left[ \mathbf{x}_1 \mathbf{1}_{\{\mathbf{x}_1^\top \mathbf{w}_r(k) \geq 0\}} \ldots \mathbf{x}_n \mathbf{1}_{\{\mathbf{x}_n^\top \mathbf{w}_r(k) \geq 0\}} \right]
\]
and the gradient of the loss function \(\Phi \mathbf{P}\) defined in eq. (6) with respect to \(\mathbf{u}\) is given by
\[
\frac{\partial \Phi \mathbf{P}(\mathbf{u})}{\partial \mathbf{u}} = -\mathbf{P}(\mathbf{y} - \mathbf{u}(k)) = -\mathbf{Pz}(k),
\]
which is a vector of length \(n\). Hence, it follows that
\[
\dot{\mathbf{w}}_r(k+1)^\top \mathbf{x}_i - \dot{\mathbf{w}}_r(k)^\top \mathbf{x}_i = \sqrt{2\eta} \frac{\mathbf{a}_r}{\sqrt{m}} \sum_{p=1}^n (\mathbf{Pz}(k))_p \mathbf{x}_i^\top \mathbf{x}_p \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k) \geq 0\}} \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k+1) \geq 0\}},
\]
where \((\mathbf{Pz}(k))_p\) denotes the \(p\)th element of \(\mathbf{Pz}(k)\). Using the property of ReLU that
\[
(b - a) \mathbf{1}_{\{a > 0\}} \leq \text{ReLU}(b) - \text{ReLU}(a) \leq (b - a) \mathbf{1}_{\{b > 0\}}, \quad a, b \in \mathbb{R},
\]
we have
\[
\text{ReLU}(\dot{\mathbf{w}}_r(k+1)^\top \mathbf{x}_i) - \text{ReLU}(\dot{\mathbf{w}}_r(k)^\top \mathbf{x}_i) \leq \sqrt{2\eta} \frac{\mathbf{a}_r}{\sqrt{m}} \sum_{p=1}^n (\mathbf{Pz}(k))_p \mathbf{x}_i^\top \mathbf{x}_p \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k) \geq 0\}} \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k+1) \geq 0\}},
\]
and
\[
\text{ReLU}(\dot{\mathbf{w}}_r(k+1)^\top \mathbf{x}_i) - \text{ReLU}(\dot{\mathbf{w}}_r(k)^\top \mathbf{x}_i) \geq \sqrt{2\eta} \frac{\mathbf{a}_r}{\sqrt{m}} \sum_{p=1}^n (\mathbf{Pz}(k))_p \mathbf{x}_i^\top \mathbf{x}_p \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k) \geq 0\}} \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k+1) \geq 0\}}.
\]
Hence, we have
\[
(\mathbf{u}(k+1))_i - (\mathbf{u}(k))_i = \sqrt{\frac{2}{m}} \sum_{r \in A} (\text{ReLU}(\dot{\mathbf{w}}_r(k+1)^\top \mathbf{x}_i) - \text{ReLU}(\dot{\mathbf{w}}_r(k)^\top \mathbf{x}_i))
- \sqrt{\frac{2}{m}} \sum_{r \in B} (\text{ReLU}(\dot{\mathbf{w}}_r(k+1)^\top \mathbf{x}_i) - \text{ReLU}(\dot{\mathbf{w}}_r(k)^\top \mathbf{x}_i))
\leq \frac{2\eta}{m} \sum_{r \in A} \sum_{p=1}^n (\mathbf{Pz}(k))_p \mathbf{x}_i^\top \mathbf{x}_p \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k) \geq 0\}} \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k+1) \geq 0\}}
+ \frac{2\eta}{m} \sum_{r \in B} \sum_{p=1}^n (\mathbf{Pz}(k))_p \mathbf{x}_i^\top \mathbf{x}_p \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k) \geq 0\}} \mathbf{1}_{\{\mathbf{x}_p^\top \mathbf{w}_r(k+1) \geq 0\}}
= 2\eta \sum_{p=1}^n \left( \hat{H}^{+}_p(k) + H^{-}_p(k) \right) (\mathbf{Pz}(k))_p.
\]
This proves the first inequality. The second inequality can be shown with a similar argument. \(\square\)

In particular, if there is no sign flip of the weights, then \(\dot{\mathbf{H}}(k) = \dot{\mathbf{H}}^{+}(k) + \dot{\mathbf{H}}^{-}(k) = \mathbf{H}(k)\) and the inequalities in Lemma 1 are equalities. Next, using Lemma 1 we can derive an expression for \(\mathbf{y} - \mathbf{u}(k)\) using \(\dot{\mathbf{H}}^{+}\), up to an error term.
Lemma 2. For any $0 < \eta < 1/(2M_I M_P n)$ and any $k \geq 0$, we have that
\[
y - u(k) = (I - 2\eta H^\infty P)^k (y - u(0)) + \epsilon(k), \tag{25}\]
where
\[
\|\epsilon(k)\|_p \leq 2\eta \sum_{t=0}^{k-1}\left(\|H^\infty - H(t)\|_p \left\| (I - 2\eta H^\infty P)^t (y - u(0)) \right\|_p + 2\eta \sum_{t=0}^{k-1} (\|M(t)\|_p + \|L(t)\|_p) \|y - u(t)\|_p. \tag{26}\n\]

Proof. For $k \geq 1$, we define $r(k)$ by
\[
r(k) = y - u(k) - (I - 2\eta H(k-1) P)(y - u(k-1)). \tag{27}\n\]
Then, by Lemma 1 we have
\[
\|r(k)\|_p \leq 2\eta \left( \|M(k-1)\|_p + \|L(k-1)\|_p \right) \|y - u(k-1)\|_p. \tag{28}\n\]
Note that eq. (27) is a first-order non-homogeneous recurrence relation for $y - u(k)$, which has an analytic solution. Thus, we can expand $y - u(k)$ for $k \geq 1$ as
\[
y - u(k) = ((I - 2\eta H(k-1) P) \cdots (I - 2\eta H(0) P)) (y - u(0)) + r(k) + \sum_{t=1}^{k-1} ((I - 2\eta H(k-1) P) \cdots (I - 2\eta H(t) P)) r(t). \tag{29}\n\]
Moreover, we can write the product of of the matrices as [Su and Yang 2019]
\[
(I - 2\eta H(k-1) P) \cdots (I - 2\eta H(0) P) = (I - 2\eta H^\infty P)^k + 2\eta (H^\infty P - H(k-1) P)(I - 2\eta H^\infty P)^{k-1} + 2\eta \sum_{t=1}^{k-1} ((I - 2\eta H(k-1) P) \cdots (I - 2\eta H(t) P)) (H^\infty P - H(t-1) P)(I - 2\eta H^\infty P)^{t-1}. \tag{30}\n\]
Combining eq. (29) and eq. (30), we obtain eq. (25) where
\[
\epsilon(k) = 2\eta (H^\infty P - H(k-1) P)(I - 2\eta H^\infty P)^{k-1} (y - u(0)) + \sum_{t=1}^{k-1} ((I - 2\eta H(k-1) P) \cdots (I - 2\eta H(t) P))(H^\infty - H(t-1)) P(I - 2\eta H^\infty P)^{t-1} (y - u(0)) + r(k) + \sum_{t=1}^{k-1} ((I - 2\eta H(k-1) P) \cdots (I - 2\eta H(t) P)) r(t).
\]
Finally, we note that
\[
\lambda_{\text{max}}(H(t) P) = \lambda_{\text{max}}(P^{1/2} H(t) P^{1/2}) = \left\| P^{1/2} H(t) P^{1/2} \right\|_2 = \sup_{\xi \in \mathbb{R}^n \setminus \{0\}} \frac{\left\| P^{1/2} H(t) P^{1/2} \xi \right\|_2}{\|\xi\|_2} = \sup_{\xi \in \mathbb{R}^n \setminus \{0\}} \frac{\left\| P^{1/2} H(t) P \xi \right\|_2}{\|\xi\|_2} = \frac{\|H(t) P\xi\|_p}{\|\xi\|_p} = \|H(t) P\|_p, \tag{31}\n\]
and that
\[
\|H(t) P\|_p = \sup_{\xi \in \mathbb{R}^n \setminus \{0\}} \frac{\|H(t) P \xi\|_p}{\|\xi\|_p} = \sup_{\xi \in \mathbb{R}^n \setminus \{0\}} \frac{\|H(t) P \xi\|_p \|H(t) P \xi\|_2}{\|\xi\|_p} = \|H(t) P\|_2. \tag{32}\n\]
We can then bound $\|H(t) P\|_p$ using $M_I$ and $M_P$ defined in eq. (8) and $\|H(t)\|_2$ as
\[
\|H(t) P\|_p \leq M_I \|H(t)\|_2 M_P \leq M_I M_P \sqrt{\|H(t)\|_1 \|H(t)\|_\infty} \leq M_I M_P n. \tag{33}\n\]
By requiring that $\eta < 1/(2M_I M_P n)$, we have $\lambda_{\text{min}}(I - 2\eta H(t) P) > 0$ for all $t$. Hence, $I - 2\eta H(t) P$ is positive definite in $(\mathbb{R}^n, \langle \cdot, \cdot \rangle_p)$, and according to eq. (31), we have $\|I - 2\eta H(t) P\|_p = \lambda_{\text{max}}(I - 2\eta H(t) P) < 1$. The upper bound in eq. (26) follows from the triangle inequality and our estimate on $r_k$ in eq. (28). \hfill \square
The residual terms in Lemma 2 can be made small by controlling \( \|M(t)P\|_p + \|L(t)P\|_p \) and \( \|(H(0) - H(t))P\|_p \). Their upper bounds are given in Lemma 3. First, we define

\[
S_i(t) = \{1 \leq r \leq m \mid 1\{\hat{w}_r(t')\mathbf{1}_i > 0\} \neq 1\{\hat{w}_r(t)\mathbf{1}_i > 0\} \text{ for some } 0 \leq t' \leq t \}
\]

to be the set of indices of the weights that have changed sign at least once by the \( k \)-th iteration.

**Lemma 3.** For all \( t \geq 0 \), we have

\[
\max (\|M(t)P\|_p + \|L(t)P\|_p, \|(H(0) - H(t))P\|_p) \leq \sqrt{\frac{4M_I^2 \beta^2\|n\|}{m^2} \sum_{i=1}^{n} |S_i(t)|},
\]

where we Moreover, for any \( 0 < \delta < 1 \), with probability at least \( 1 - \delta \), we have

\[
\|(H^\infty - H(0))P\|_p \leq 2M_I \beta n \sqrt{\log(2n/\delta)}.
\]

**Proof.** First, we have

\[
\|M(t)P\|_p^2 \leq M_I^2 \beta^2 \|M(t)\|_2^2 \leq M_I^2 \beta^2 \|M(t)\|_F^2 \\
\leq \frac{M_I^2 \beta^2}{m^2} \sum_{i=1}^{n} \sum_{p=1}^{m} \left( \sum_{r \in A} \|1\{\hat{w}_r(t')\mathbf{1}_i > 0, \hat{w}_r(t)\mathbf{1}_i > 0\} - 1\{\hat{w}_r(t)\mathbf{1}_i > 0, \hat{w}_r(t')\mathbf{1}_i > 0\} \right)^2 \leq \frac{M_I^2 \beta^2}{m^2} \sum_{i=1}^{n} |S_i(t)|^2.
\]

The estimate for \( \|L(t)P\|_p^2 \) is exactly the same and obtained by replacing \( A \) with \( B \). We also have

\[
\|(H(0) - H(t))P\|_p^2 \leq M_I^2 \beta^2 \|H(0) - H(t)\|_2^2 \leq M_I^2 \beta^2 \|H(0) - H(t)\|_F^2 \\
\leq \frac{M_I^2 \beta^2}{m^2} \sum_{i=1}^{n} \sum_{p=1}^{m} \left( \sum_{r \in A} \|1\{\hat{w}_r(t')\mathbf{1}_i > 0, \hat{w}_r(t)\mathbf{1}_i > 0\} - 1\{\hat{w}_r(t)\mathbf{1}_i > 0, \hat{w}_r(t')\mathbf{1}_i > 0\} \right)^2 \leq \frac{M_I^2 \beta^2}{m^2} \sum_{i=1}^{n} |S_i(t)| + |S_p(t)| \leq \frac{M_I^2 \beta^2}{m^2} \sum_{i=1}^{n} \sum_{p=1}^{n} \left( 2|S_i(t)|^2 + 2|S_p(t)|^2 \right) \leq \frac{4M_I^2 \beta^2}{m^2} \sum_{i=1}^{n} |S_i(t)|^2.
\]

This proves the first inequality. Since \( H_{ij}(0) \) is the average of \( m \) iid random variables bounded in \([0,1]\), by Hoeffding’s inequality [Hoeffding, 1963], for any \( t > 0 \) and any \( 1 \leq i, j \leq n \), we have

\[
\mathbb{P}\left( \frac{1}{m} \left| H_{ij}(0) - H_{ij}^\infty \right| \geq t \right) \leq 2 \exp \left( -\frac{2t^2}{m} \right) \leq 2 \exp \left( -\frac{t^2}{m} \right).
\]

Set \( t = \sqrt{\frac{\log(2n^2/\delta)}{m}} \). With probability at least \( 1 - \delta/n^2 \), we have

\[
\left| H_{ij}(0) - H_{ij}^\infty \right| \leq \sqrt{\frac{\log(2n^2/\delta)}{m}} \leq 2 \sqrt{\frac{\log(2n/\delta)}{m}}.
\]

Hence, by a union bound, we know that with probability at least \( 1 - \delta \), we have

\[
\|H^\infty - H(0)\|_2 \leq \|H^\infty - H(0)\|_F \leq 2n \sqrt{\frac{\log(2n/\delta)}{m}}.
\]

The last estimate follows from the definitions of \( M_I \) and \( M_P \) (see eq. (8) and eq. (32)).
Lemma 4. Let $\epsilon > 0, \kappa > 0, 0 < \delta < 1$ and $T > 0$ be given. There exist constants $C_m, C'_m > 0$ such that if $0 \leq \eta \leq 1/(2M_1M_Pn)$ and $m$ satisfies
\[
m \geq C_m \frac{M^2 M_P n^3}{\kappa^2 \epsilon^2} \left( \lambda_0^{-4} \left( 1 + \frac{\kappa^2 M^2_1 n}{\delta} \right)^2 + \eta^4 T^4 \epsilon^4 \right)
\]
and
\[
m \geq C'_m \frac{M^2 M_P n^2 \log(n/\delta)}{\epsilon^2} \left( \frac{\lambda_0^{-2}}{1 + \frac{\kappa^2 M^2_1 n}{\delta}} + \eta^2 T^2 \epsilon^2 \right),
\]
then with probability at least $1 - \delta$, we have the following for all $0 \leq k \leq T$:
\[
y - u(k) = (I - 2\eta H^\infty)^k (y - u(0)) + \epsilon(k), \quad \|\epsilon(k)\|_P \leq \epsilon.
\](35)

Proof. Set $\delta' = \delta/3$. For any $R > 0$ and $r = 1, \ldots, m$, since $w_r(0)^\top x_i \sim N(0, \kappa^2)$, we have
\[
P \left( |\tilde{w}_r(0)^\top x_i| \leq R \right) = \mathbb{E} \left[ |w_r(0)^\top x_i| \leq R \right] < \frac{2R}{\sqrt{\pi} R}.
\]
By Hoeffding’s inequality [Hoeffding, 1963], for any $t > 0$ we have
\[
P \left( \sum_{r=1}^{m} \mathbb{1}_{\{w_r(0)^\top x_i \leq t\}} \geq 2mR \frac{\sqrt{\log(n/\delta')}}{\sqrt{\pi} R} \right) \leq \exp \left( - \frac{2\log(n/\delta')}{m} \right), \quad 1 \leq i \leq n.
\] (36)
Thus, if we set $t = \sqrt{m \log(n/\delta')}$ then we find that with probability at least $1 - \delta'/n$ we have
\[
\sum_{r=1}^{m} \mathbb{1}_{\{w_r(0)^\top x_i \leq R\}} \leq 2mR \frac{\sqrt{\log(n/\delta')}}{\sqrt{\pi} R} + \sqrt{m \log(n/\delta')}. \leq 2m \left( R \frac{\sqrt{\log(n/\delta')}}{\sqrt{\pi} R} + \frac{\sqrt{\log(n/\delta')}}{m} \right).
\]
By a union bound, we have with probability at least $1 - \delta'$,
\[
\sum_{i=1}^{n} \left( \sum_{r=1}^{m} \mathbb{1}_{\{w_r(0)^\top x_i \leq R\}} \right)^2 \leq 4m^2 \left( R \frac{\sqrt{\log(n/\delta')}}{\sqrt{\pi} R} + \frac{\sqrt{\log(n/\delta')}}{m} \right)^2.
\]
By combining this with Lemma 3 we have that with probability at least $1 - 2\delta'$,
\[
\sqrt{\frac{4M^2 M_P^2 n}{\epsilon^2}} \sum_{i=1}^{n} \left( \sum_{r=1}^{m} \mathbb{1}_{\{w_r(0)^\top x_i \leq R\}} \right)^2 \leq 4M_1M_Pn \left( R \frac{\sqrt{\log(n/\delta')}}{\sqrt{\pi} R} + \frac{\sqrt{\log(n/\delta')}}{m} \right), \quad \sum_{i=1}^{n} \mathbb{1}_{\{w_r(0)^\top x_i \leq R\}} = \mathbb{1}_{\{w_r(0)^\top x_i \leq R\}}.
\] (37)
and
\[
\| (H^\infty - H(0)) \|_P \leq 2M_1M_Pn \sqrt{\frac{\log(2n/\delta')}{m}}.
\] (38)
Since the $i$th entry of $u(0)$ has mean 0 and variance $\leq \kappa^2$, we have $\mathbb{E}[(u(0))^2] \leq \kappa^2$, where $(u(0))_i$ is the $i$th entry. Hence, we have $\mathbb{E} \left[ \|u(0)\|_P^2 \right] \leq M_1^2 n \kappa^2$. By Markov’s inequality, with probability at least $1 - \delta'$, we have
\[
\|u(0)\|_P \leq \kappa M_1 \sqrt{n/\delta'}, \quad \|y - u(0)\|_P \leq \|y\|_P + \kappa M_1 \sqrt{n/\delta'}.
\] (39)
By a union bound, we know that eqs. (37) to (39) hold with probability of at least $1 - 3\delta'$. The theorem now follows using induction, where the base case when $k = 0$ is obvious. Assume eq. (35) holds for $t = 0, \ldots, k - 1$, where $1 \leq k \leq T$. Then, we have
\[
2n \sum_{t=0}^{k-1} \|y - u(t)\|_P \leq 2n \sum_{t=0}^{k-1} \left( (1 - 2\eta \lambda_0)^t \|y - u(0)\|_P + \epsilon \right) \leq \lambda_0^{-1} \|y - u(0)\|_P + 2\eta T \epsilon,
\] (40)
where the first inequality follows from the fact that $I - 2\eta H^\infty P$ is positive semidefinite in $(\mathbb{R}^n, \langle \cdot, \cdot \rangle_P)$ with the maximum eigenvalue being $1 - 2\eta \lambda_0$, and the second inequality follows by bounding the power series. By the definition of $\lambda_0$, we have
\[
2n \sum_{t=0}^{k-1} \left( (I - 2\eta H^\infty P)^t (y - u(0)) \right) \|_P \leq 2n \sum_{t=0}^{k-1} (1 - 2\eta \lambda_0)^t \|y - u(0)\|_P \leq \lambda_0^{-1} \|y - u(0)\|_P.
\] (41)
By Lemma $2$ and $3$, we have

\[ y - u(k) = (I - 2\eta H^\infty P)^k (y - u(0)) + \epsilon(k) \]

with

\[ \|\epsilon(k)\|_P \leq \lambda_0^{-1} \|([H(0) - H^\infty] P)\|_P \|y - u(0)\|_P + 2 \sqrt{\frac{4M_1^2 M_2^2 n}{m^2} \sum_{i=1}^n |S_i(k)|^2 (\lambda_0^{-1} \|y - u(0)\|_P + \eta T\epsilon)}, \tag{42} \]

where we used the fact that \(|S_i(t)|\) is a nondecreasing function of \(t\) and the triangle inequality \|

\[ \|([H^\infty - H(t)] P)\|_P \leq \|([H(0) - H^\infty] P)\|_P + \|H(t) - H(0)\|_P. \]

Here, we also combined \(\lambda_0^{-1} \|([H(t) - H(0)] P)\|_P \|y - u(0)\|_P\) with the last term on the right-hand side of eq. (26) and applied Lemma $3$, eq. (40), and eq. (41) to obtain the last term on the right-hand side of eq. (42). To control \(|S_i(k)|\), we first bound the change of the weights. For any \(0 \leq t \leq k - 1\) and \(1 \leq r \leq m,\) the change of weights in one iteration can be bounded by

\[ \|\acute{w}_r(t + 1) - \acute{w}_r(t)\|_2 \leq \eta \left\| \frac{\partial u(t)}{\partial \acute{w}_r} \right\|_F \left\| P(y - u(t)) \right\|_2 \leq \eta \sqrt{\frac{2n}{m}} M_P \|y - u(t)\|_P, \]

where the inequalities follow from eq. (23) and eq. (24). Hence, the total change of the weights can be bounded by

\[ \|\acute{w}_r(t) - \acute{w}_r(0)\|_2 \leq \eta M_P \sqrt{\frac{2n}{m}} \sum_{t'=0}^{t-1} \|y - u(t')\|_P \leq R_T, \tag{43} \]

where \(R_T = M_P \sqrt{\frac{2n}{m}} (\lambda_0^{-1} \|y - u(0)\|_P + 2\eta T\epsilon).\) Recall that \(S_i(k)\) is the set of indices of weights that have gone through at least one sign flip by iteration \(k.\) Thus, if \(r \in S_i(k),\) we have \(|\acute{w}_r(t) - \acute{w}_r(0)\|_2 \geq |\acute{w}_r(0)\|_2 |x_i|\) for some \(0 \leq t \leq k\) as the sign flip leads to \(|\acute{w}_r(0)\|_2 |x_i| \leq |\acute{w}_r(t)\|_2 |x_i|).\) This gives us

\[ |S_i(k)| \leq \left\{ \{r \in [m] : |\acute{w}_r(0)\|_2 |x_i| \leq \|\acute{w}_r(t) - \acute{w}_r(0)\|_2 \text{ for some } 0 \leq t \leq k \} \right\}, \tag{44} \]

where \([m] = \{1, \ldots, m\}.\) Hence, there exists a constant \(C > 0\) such that

\[ \|\epsilon(k)\|_P \leq 2M_1 M_P n \sqrt{\frac{\log(2n/\delta)}{m}} \lambda_0^{-1} \|y - u(0)\|_P + 8M_1 M_P n \left( \frac{R_T}{\sqrt{\pi \kappa}} + \sqrt{\frac{\log(n/\delta)}{m}} \right) (\lambda_0^{-1} \|y - u(0)\|_P + \eta T\epsilon) \]

\[ \leq 2M_1 M_P n \left( \frac{\log(6n/\delta)}{m} \lambda_0^{-1} C \left( 1 + \kappa M_1 \sqrt{\frac{3n}{\delta}} \right) \left( 1 + \kappa M_1 \sqrt{\frac{3n}{\delta}} \right) + 2\eta T\epsilon \right) \]

\[ \times \left( \lambda_0^{-1} C \left( 1 + \kappa M_1 \sqrt{\frac{3n}{\delta}} \right) + \eta T\epsilon \right), \]

where the first inequality follows from eq. (37), eq. (42), and eq. (44), and the second inequality follows from eq. (39) and eq. (43). Finally, eq. (35) follows from the way we define \(m.\) By taking \(C_m,\) large enough, we guarantee that \(2M_1 M_P n A_1, 8M_1 M_P n A_2 A_4 < \epsilon/3.\) By taking \(C'_m\) large enough, we guarantee that \(8M_1 M_P n A_3 A_4 < \epsilon/3.\) Hence, eq. (35) follows. \(\square\)
Lemma 4 gives us an estimate of the residual \( y - u(k) \) in terms of the initial residual \( y - u(0) \). However, in analyzing the frequency bias, we hope to express the residual in terms of \( y \) only. This can be done by controlling the size of \( u(0) \). First, we note that the proof of eq. 39 does not rely on the assumptions on \( m \) in Lemma 4. Hence, it holds for any \( n, m \geq 1, \kappa > 0, 0 < \delta < 1 \), and positive definite matrix \( P \). Now we are ready to prove our first main result Theorem 1.

Proof of Theorem 1 By eq. (39), with probability at least \( 1 - \delta / 2 \), we have

\[
\left\lVert (I - \eta H^\infty P)^k u(0) \right\rVert_P \leq \left\lVert u(0) \right\rVert_P \leq \kappa M_1 \sqrt{2n/\delta}.
\]

By taking \( \kappa \leq \epsilon \sqrt{\delta / 2n}/(2M_1) \), we guarantee that

\[
\left\lVert (I - \eta H^\infty P)^k u(0) \right\rVert_P \leq \epsilon / 2.
\]

By the way we pick \( \kappa \) and \( m \), for some constant \( C' > 0 \) that only depends on \( d \), we have

\[
1 + \frac{\kappa^2 M_1^2 n}{\delta} \leq C'.
\]

Hence, by taking \( C_2 \) in eq. 12 large enough, we guarantee that \( m \) satisfies the assumptions in Lemma 4 with \( \epsilon \), \( \kappa \), \( T \), and \( \delta \) to be \( \epsilon / 2 \), \( \kappa \), \( T \), and \( \delta / 2 \), respectively. Then, we have eq. 45 is true with probability of at least \( 1 - \delta / 2 \), for which \( \| \epsilon (k) \|_P \leq \epsilon / 2 \). The result follows from the triangle inequality and union bound.

Notably, there are other initialization schemes that allow us to avoid using \( \kappa \). One of the examples is to initialize the weights at odd indices \( w_{2p+1} \) and \( a_{2p+1} \) randomly and set \( w_{2p+2} = w_{2p+1} \), \( a_{2p+2} = -a_{2p+1} \), assuming \( m \) is even [Su and Yang, 2019]. This initialization scheme guarantees that \( u(0) = 0 \) and hence we do not need to introduce \( \kappa \) to control the initialization size \( \| u(0) \|_P \).

D The theory of frequency biasing with an \( L^2 \)-based loss function

In this section, we prove the results stated in Section 4, where we are concerned with the frequency biasing behavior of NN training when using the squared \( L^2 \) norm as the loss function. We theoretically show the frequency biasing phenomena in this setting, up to a quadrature error.

D.1 A consequence of Theorem 1

Given a bandlimited function \( g : S^{d-1} \rightarrow \mathbb{R} \) with bandlimit \( L \), we can uniquely decompose \( g \) into a spherical harmonic expansion as \( g(x) = \sum_{\ell=0}^{L} g_{\ell}(x) \), where \( g_{\ell}(x) \in \mathcal{H}_\ell^d \). Here, \( \mathcal{H}_\ell^d \) is the space of the restriction of (real) homogeneous harmonic polynomials of degree \( \ell \) on \( S^{d-1} \). That is,

\[
g_{\ell}(x) = \sum_{p=1}^{N(d, \ell)} \hat{g}_{\ell,p} Y_{\ell,p}, \quad \hat{g}_{\ell,p} = \int_{S^{d-1}} g(x) Y_{\ell,p}(x) dx.
\]

where \( N(d, \ell) \) is given in section 2 and \( Y_{\ell,p} \) are the spherical harmonic function of degree \( \ell \) and order \( p \). As a consequence of Theorem 1, we can consider the NN training error with the squared \( L^2 \)-based loss function.

Proof of Theorem 2 By Theorem 1 for every \( k = 0, \ldots, T \), we can write

\[
\| u(k) - y \|_c = \| (I - 2\eta H^\infty D_c)^k y \|_c + \varepsilon_3(k), \quad \| \varepsilon_3(k) \|_c \leq \| \epsilon(k) \|_c \leq \epsilon.
\]

To estimate the first term, we first note that the matrix \( I - 2\eta H^\infty D_c \) is positive semidefinite in \( (\mathbb{R}^n, \langle \cdot, \cdot \rangle_c) \) and \( \| I - 2\eta H^\infty D_c \|_c \leq 1 - 2\eta \lambda_0 \) (see Theorem 1). Since \( g(x) = \sum_{\ell=0}^{L} g_{\ell}(x) \), we have

\[
(I - 2\eta H^\infty D_c)^k y = \sum_{\ell=0}^{L} (I - 2\eta H^\infty D_c)^k y^\ell, \quad y = \sum_{\ell=0}^{L} y^\ell,
\]
where \( y^\ell = [g_\ell(x_1), \ldots, g_\ell(x_n)]^T \in \mathbb{R}^n \). By the Funk–Hecke formula and the quadrature rule, we have

\[
(H^\infty D_c y^\ell)_p = \sum_{i=1}^{n} c_i K^\infty(x_p, x_i) g_\ell(x_i) = \int_{\mathbb{R}^{d-1}} K^\infty(x_p, \xi) g_\ell(\xi) d\xi + e_{p,\ell}^d = \mu_\ell g_\ell(x_p) + e_{p,\ell}^d,
\]

where \( e_{p,\ell}^d \) is a quadrature error (see eq. (15)). Therefore, in vectorized form, we have \( H^\infty D_c y^\ell = \mu_\ell y^\ell + e_{\ell}^d \) or, equivalently, \( (I - 2\eta H^\infty D_c) y^\ell = (1 - 2\eta \mu_\ell) y^\ell - 2\eta e_{\ell}^d \), where \( e_{\ell}^d = (e_{1,\ell}^d, \ldots, e_{n,\ell}^d)^T \).

By applying \( I - 2\eta H^\infty D_c \) to \( y^\ell \) for \( k \) times, we find that

\[
(I - 2\eta H^\infty D_c)^k y^\ell = (1 - 2\eta \mu_\ell)^k y^\ell - 2\eta \sum_{t=0}^{k-1} (1 - 2\eta \mu_\ell)^t (I - 2\eta H^\infty D_c)^{k-t-1} e_{\ell}^d.
\]

The second term, \( e_{\ell}^d \), can be easily bounded from above to obtain

\[
\|e_{\ell}^d\|_c \leq 2\eta \|e_{\ell}^d\|_c \sum_{t=0}^{\infty} (1 - 2\eta \mu_\ell)^t = \frac{1}{\mu_\ell} \|e_{\ell}^d\|_c.
\]

The inequality above shows that \( (I - 2\eta H^\infty D_c)^k y^\ell \) is close to \( (1 - 2\eta \mu_\ell)^k y^\ell \). We define

\[
\varepsilon_2 = \left\| \sum_{\ell=0}^{L} (I - 2\eta H^\infty D_c)^k y^\ell \right\|_c - \left\| \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell)^k y^\ell \right\|_c
\]

to be the quantity in the statement of Theorem 2 which measures the accuracy of approximating the eigenvalues and eigenvectors of \( H^\infty D_c \) using the eigenvalues and eigenfunctions of the continuous kernel \( K^\infty \). Hence, we have

\[
\left\| (I - 2\eta H^\infty D_c)^k y^\ell \right\|_c = \left\| \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell)^k y^\ell \right\|_c + \varepsilon_2.
\]

Using the triangle inequality, we have

\[
\varepsilon_2 \leq \sum_{\ell=0}^{L} \left\| e_{\ell}^d \right\|_c \leq \sum_{\ell=0}^{L} \frac{1}{\mu_\ell} \left\| e_{\ell}^d \right\|_c = \sum_{\ell=0}^{L} \frac{1}{\mu_\ell} \left[ \sum_{i=1}^{n} c_i (e_{i,\ell}^d)^2 \right] \leq \sum_{\ell=0}^{L} \frac{\sqrt{A_d}}{\mu_\ell} \max_{1 \leq i \leq n} |c_i|.
\]

Recall that \( \sum_{i=1}^{n} c_i = A_d \), the surface area of \( \mathbb{S}^{d-1} \). Next, we can write

\[
\left\| \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell)^k y^\ell \right\|_c^2 = \left( \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell)^k y^\ell \right)^T D_c \left( \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell)^k y^\ell \right)
\]

\[
= \sum_{\ell=0}^{L} \sum_{j=0}^{L} (1 - 2\eta \mu_j)^k (1 - 2\eta \mu_\ell)^k y^\ell y^\ell^T D_c y^\ell
\]

\[
= \sum_{\ell=0}^{L} \sum_{j=0}^{L} (1 - 2\eta \mu_j)^k (1 - 2\eta \mu_\ell)^k \left( \int_{\mathbb{S}^{d-1}} g_j(\xi) g_\ell(\xi) d\xi + e_{j,\ell}^c \right)
\]

\[
= \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell)^{2k} \| g_\ell \|_2^2 + \sum_{j=0}^{L} \sum_{\ell=0}^{L} (1 - 2\eta \mu_j)^k (1 - 2\eta \mu_\ell)^k e_{j,\ell}^c
\]

(47)

where we used the fact that \( g_j \) and \( g_\ell \) are orthogonal in \( L^2(\mathbb{S}^{d-1}) \) for \( j \neq \ell \). Combining eq. (46) and eq. (47), we can write

\[
\left\| (I - 2\eta H^\infty D_c)^k y^\ell \right\|_c = \sqrt{\sum_{j=0}^{L} (1 - 2\eta \mu_j)^{2k} \| g_j \|_2^2} + \varepsilon_1(k) + \varepsilon_2,
\]

(48)
where
\[ |\varepsilon_1(k)| \leq \sum_{j=0}^{L} \sum_{\ell=0}^{L} (1 - 2\eta\mu_j)^k (1 - 2\eta\mu_\ell)^k c_{j,\ell}. \]

The result follows from eq. (45) and eq. (48).

**D.2 Frequency biasing up to an approximation error**

Theorem 2 shows that we theoretically have frequency biasing up to the level of quadrature errors \( \varepsilon_1(k) \) and \( \varepsilon_2 \). If the quadrature errors are large, then we may not observe frequency biasing in practice. Here, we show that the quadrature errors can be made arbitrarily small by taking enough samples in the training data. Recall that our quadrature rule satisfies eq. (17).

Next, we pass the quadrature error to the approximation error, which may not necessarily be tight. However, this allows us to use the existing theory of spherical harmonics approximation to show the decay of quadrature errors.

**Lemma 5.** Let \( f : \mathbb{S}^{d-1} \to \mathbb{R} \) be a function and \( \text{dist}(f, \Pi_\ell^d) = \min_{h \in \Pi_\ell^d} \| f - h \|_{L^\infty} \). We have
\[
\left| \int_{\mathbb{S}^{d-1}} f(\xi) d\xi - \sum_{i=1}^{n} c_i f(x_i) \right| \leq 2\gamma_n,\ell \| f \|_{L^\infty} + 2A_d \text{dist}(f, \Pi_\ell^d) \tag{49}
\]
for any integer \( \ell \geq 0 \).

**Proof.** Let \( h_\ell = \arg \min_{h \in \Pi_\ell^d} \| f - h \|_{L^\infty} \). By the triangle inequality, we have
\[
\left| \int_{\mathbb{S}^{d-1}} f(\xi) d\xi - \sum_{i=1}^{n} c_i f(x_i) \right| \\
\leq \left| \int_{\mathbb{S}^{d-1}} f(\xi) d\xi - \int_{\mathbb{S}^{d-1}} h_\ell(\xi) d\xi \right| + \left| \int_{\mathbb{S}^{d-1}} h'_\ell(\xi) d\xi - \sum_{i=1}^{n} c_i h'_\ell(x_i) \right| + \sum_{i=1}^{n} c_i (h'_\ell(x_i) - f(x_i)) \\
\leq A_d \text{dist}(f, \Pi_\ell^d) + \gamma_n,\ell \| h_\ell \|_{L^\infty} + A_d \text{dist}(f, \Pi_\ell^d) \leq 2\gamma_n,\ell \| f \|_{L^\infty} + 2A_d \text{dist}(f, \Pi_\ell^d),
\]
where we used the fact that \( c_i > 0 \) for \( i = 1, \ldots, n \) and the fact that \( \| h_\ell \|_{L^\infty} \leq 2 \| f \|_{L^\infty} \).

Next, we focus on controlling the minimum approximation error \( \text{dist}(f, \Pi_\ell^d) \) on the right-hand side of eq. (49). To do so, we prove the following lemma.

**Lemma 6.** Let \( f(\xi) = K^\infty(x_i, g_j(\xi)) \) and \( g(\xi) = g_j(\xi)g_p(\xi) \). Then, for a constant \( C > 0 \) that only depends on \( d \), we have
\[
\text{dist}(f_{ij}, \Pi_\ell^d) \leq C \frac{j + 1}{\ell} \| g_j \|_{L^\infty}, \quad 1 \leq i \leq n, 0 \leq j \leq L,
\]
\[
\text{dist}(g_{jp}, \Pi_\ell^d) \leq C \frac{j + p}{\ell} \| g_j \|_{L^\infty} \| g_p \|_{L^\infty}, \quad 0 \leq j, p \leq L,
\]
for all \( \ell \geq 1 \).

**Proof.** For \( 1 \leq a < b \leq d \) where \( a, b \in \mathbb{N} \), and \( t \in [-\pi, \pi] \), let \( Q_{a,b,t} \) denote the action on \( \mathbb{S}^{d-1} \) of rotation by the angle \( t \) in the \( (x_a, x_b) \)-plane. For an integer \( \alpha \geq 1 \), we define the operator on functions on \( \mathbb{S}^{d-1} \) by
\[
\Delta_{a,b,t}^\alpha = (I - T(Q_{a,b,t}))^\alpha,
\]
where \( T(Q)f(x) = f(Q^{-1}x) \). If \( f \in C(\mathbb{S}^{d-1}) \), then we define for \( t > 0 \) that
\[
\omega_\alpha(f; t) = \max_{1 \leq a < k \leq d} \sup_{|\theta| \leq t} \| \Delta_{a,b,t}^\alpha f \|_{L^\infty}.
\]
By [Dai and Xu 2013, Thm. 4.4.2], we have
\[
\text{dist}(f, \Pi_\ell^d) \leq c_1 \omega_\alpha(f; \ell^{-1}), \quad \ell \geq 1, \alpha \geq 1,
\]
where \( c_1 > 0 \) is some constant that only depends on \( \alpha \). Then it is sufficient to bound \( \omega_\alpha(f_{ij}; \ell^{-1}) \) and \( \omega_\alpha(g_{ij}; \ell^{-1}) \) to finish the proof.

First, we aim to bound the term \( \text{dist}(f_{ij}, \Pi^i_j) \) where \( f_{ij}(\xi) = K^\infty(x_i, \xi)g_j(\xi) \). We fix \( 1 \leq i \leq n, 1 \leq a < b \leq d \) where \( i, a, b \in \mathbb{N} \), and choose \( \theta \) such that \( |\theta| \leq \ell^{-1} \). We have

\[
\| \Delta^a_{a,b,\theta} f_{ij} \|_{L^\infty} = \| f_{ij}(\xi) - f_{ij}(Q_a^{-1}_{a,b,\theta} \xi) \|_{L^\infty}.
\]

We then define

\[
\delta K_i^\infty(\xi) := K^\infty(x_i, Q_a^{-1}_{a,b,\theta} \xi) - K^\infty(x_i, \xi),
\]

\[
\delta g_j(\xi) := g_j(Q_a^{-1}_{a,b,\theta} \xi) - g_j(\xi).
\]

Next, we control the first term of eq. (50) by

\[
\| \delta g_j(\xi) \|_{L^\infty} = \| \Delta^a_{a,b,\theta} g_j(\xi) \|_{L^\infty} \leq c_2 \ell^{-1} \| D_{a,b} g_j(\xi) \|_{L^\infty} \leq c_2 \ell^{-1} \| g_j \|_{L^\infty},
\]

where \( D_{a,b} := \partial_x \partial_y - \partial_y \partial_x \) and the two inequalities follow from [Dai and Xu, 2013, Lem. 4.2.2 (iii)] and [Dai and Xu, 2013, Lem. 4.2.4], respectively. Next, we control the first term of eq. (50) by writing

\[
\| \delta K_i^\infty(\xi) (g_j(\xi) + \delta g_j(\xi)) \|_{L^\infty} \leq \| \delta K_i^\infty(\xi) \|_{L^\infty} \| g_j(Q_a^{-1}_{a,b,\theta} \xi) \|_{L^\infty} = \| \delta K_i^\infty(\xi) \|_{L^\infty} \| g_j \|_{L^\infty}.
\]

We fix \( \xi \) and define \( \xi' = Q_a^{-1}_{a,b,\theta} \xi \). It follows that

\[
\delta K_i^\infty(\xi) = K^\infty(x_i, \xi') - K^\infty(x_i, \xi)
\]

\[
= \frac{1}{4\pi} \left[ (x_i^\top \xi' + 1) \left( \pi - \arccos(x_i^\top \xi') \right) - (x_i^\top \xi + 1) \left( \pi - \arccos(x_i^\top \xi) \right) \right]
\]

\[
= \frac{1}{4\pi} \left[ x_i^\top (\xi' - \xi) \left( \pi - \arccos(x_i^\top \xi) \right) - (x_i^\top \xi' + 1) \left( \arccos(x_i^\top \xi') - \arccos(x_i^\top \xi) \right) \right]
\]

Next, by the triangle inequality for angles, we have

\[
| \arccos(x_i^\top \xi') - \arccos(x_i^\top \xi) | \leq |\theta| \leq \ell^{-1}.
\]

Since \( \arccos \) is monotone and \( |(d/dt)\arccos(t)| > 1 \) for all \( t \), by the fundamental theorem of calculus, we must have

\[
|x_i^\top \xi' - x_i^\top \xi| \leq | \arccos(x_i^\top \xi') - \arccos(x_i^\top \xi) | \leq \ell^{-1}.
\]

As a result, we have

\[
| \delta K_i^\infty(\xi) | \leq \frac{1}{4\pi} \left[ \ell^{-1} \pi + 2\ell^{-1} \right] = \frac{\pi + 2}{4\pi} \ell^{-1}.
\]

By eq. (54) and eq. (55), we find that

\[
\| \delta K_i^\infty(\xi) (g_j(\xi) + \delta g_j(\xi)) \|_{L^\infty} \leq \frac{\pi + 2}{4\pi} \ell^{-1} \| g_j \|_{L^\infty}.
\]

Putting eqs. (50) to (52) and (55) together, we obtain

\[
\| \Delta^a_{a,b,\theta} f_{ij} \|_{L^\infty} = \| f_{ij}(\xi) - f_{ij}(Q_a^{-1}_{a,b,\theta} \xi) \|_{L^\infty} \leq \left( c_2 j + \frac{\pi + 2}{4\pi} \right) \ell^{-1} \| g_j \|_{L^\infty}.
\]

Since \( a, b, \) and \( \theta \) are chosen arbitrarily, this bound also holds for \( \omega_1(f_{ij}; \ell^{-1}) \).
Second, we aim to bound the term \( \text{dist}(g_{jp}, \Pi^j_L) \) where \( g_{jp}(\xi) = g_j(\xi) g_p(\xi) \). As before, we fix the indices \( a, b \in \mathbb{N} \) where \( 1 \leq a < b \leq d \) and \( \theta \) such that \( |\theta| \leq \ell^{-1} \). Similarly, we define
\[
\delta g_j(\xi) = g_j(Q^{-1}_{a,b,\theta} \xi) - g_j(\xi), \quad \delta g_p(\xi) = g_p(Q^{-1}_{a,b,\theta} \xi) - g_p(\xi).
\]

By eq. (52), we have
\[
\left\| g_j g_p(\xi) - g_j g_p(Q^{-1}_{a,b,\theta} \xi) \right\|_{L^\infty} = \left\| g_j(\xi) g_p(\xi) - (g_j(\xi) + \delta g_j(\xi))(g_p(\xi) + \delta g_p(\xi)) \right\|_{L^\infty} \\
\leq \left\| \delta g_j(\xi)(g_p(\xi) + \delta g_p(\xi)) \right\|_{L^\infty} + \left\| g_j(\xi) \delta g_p(\xi) \right\|_{L^\infty} \\
\leq c_2 \frac{j + p}{\ell} \|g_j\|_{L^\infty} \|g_p\|_{L^\infty}.
\]

Since \( a, b, \) and \( \theta \) are arbitrary numbers, this bound also holds for \( \omega_1(g_{jp}; \ell^{-1}) \).

Using these lemmas, we can prove that Theorem 3 asymptotically controls the quadrature errors.

**Proof of Theorem 3.** First, we control \( \epsilon_1(k) \) as
\[
|\epsilon_1(k)| \leq \left| \sum_{j=0}^L \sum_{p=0}^L (1 - 2\eta \mu_j)^k (1 - 2\eta \mu_p)^k c_{jp} \right| \leq \left| \sum_{j=0}^L \sum_{p=0}^L c_{jp} \right| \\
\leq \sum_{j=0}^L \sum_{p=0}^L \left| 2\gamma_{n,\ell} \|g_{jp}\|_{L^\infty} + 2A_d \text{dist}(g_{jp}, \Pi^j_L) \right| \\
\leq \sum_{j=0}^L \sum_{p=0}^L \left( 2\gamma_{n,\ell} \|g_j\|_{L^\infty} \|g_p\|_{L^\infty} + 2A_d C \frac{j + 1}{\ell} \|g_j\|_{L^\infty} \|g_p\|_{L^\infty} \right),
\]

where the third and the forth inequalities follow from Lemma 5 and Lemma 6 respectively. The final upper bound for \( |\epsilon_1(k)| \) holds since \( \sum_{j=0}^L \sum_{p=0}^L (j + p) = O(L^3) \). Next, there exists \( C_2 > 0 \) such that we can control \( \epsilon_2 \) by writing
\[
|\epsilon_2| \leq \sum_{j=0}^L \sqrt{A_d} \mu_j \max_{1 \leq \ell \leq n} |c_{ij}| \leq \sum_{j=0}^L \sqrt{A_d} \mu_j \left( 2\gamma_{n,\ell} \|g_j\|_{L^\infty} + 2A_d C \frac{j + 1}{\ell} \|g_j\|_{L^\infty} \right) \\
\leq C_2 \left( \sum_{j=0}^L \mu_j^{-1} \right) \left( \frac{L^2}{\ell} + L\gamma_{n,\ell} \right) \max_{j} \|g_j\|_{L^\infty},
\]

where the second and the third inequalities follow from Lemma 5 and Lemma 6 respectively. The proof is complete.

**Proof of Corollary 7.** By Theorem 3 it suffices to show that \( \max_{0 \leq j \leq L} \|g_j\|_{L^\infty} \leq C \|g\|_{L^2} \) for some constant \( C > 0 \) that does not depend on \( g \). Since \( \mathcal{H}^i_L \perp \mathcal{H}^j_L \) in \( L^2 \) for \( i \neq j \), we have \( \|g_j\|_{L^2} \leq \|g\|_{L^2} \) for \( 0 \leq j \leq L \). The claim follows from the fact that \( \|\cdot\|_{L^2} \) and \( \|\cdot\|_{L^\infty} \) are equivalent in \( \Pi^j_L \).

E The theory of frequency biasing with a \( H^s \)-based loss function

This section presents detailed proofs for Proposition 2 and Theorem 4 in Section 5 which concerns the frequency biasing behavior of NN training using the \( H^s \) loss function.

E.1 A 2-layer ReLU neural network is in \( H^s(\mathbb{S}^{d-1}) \) for \( s < 3/2 \)

We prove that a 2-layer ReLU NN map is contained in \( H^s(\mathbb{S}^{d-1}) \) for any \( s < 3/2 \) (see Proposition 2).
Proof of Proposition 2. Since $N$ can be written as

$$N(x) = \sum_{r=1}^{m} a_r \text{ReLU}(w_r^T x + b_r),$$

it suffices to prove that $f(x) = \text{ReLU}(w^T x + b)$ is in $H^s$ for all $w \in \mathbb{R}^d, b \in \mathbb{R}$. Since $\text{ReLU}(ax) = a\text{ReLU}(x)$ for any $a > 0$, we can assume that $\|w\|_2 = 1$. Moreover, since the Sobolev spaces are rotationally invariant, we can assume that $w = (1, 0, \ldots, 0)^T$. Then, $f$ can be written as

$$f(x) = \text{ReLU}(x_1 + b).$$

If $b \leq -1$ or $b \geq 1$, then $f(x)$ is a constant, and thus $f \in H^s(\mathbb{S}^{d-1})$ for all $s \in \mathbb{R}$. We assume $-1 < b < 1$. Then, we have

$$f(x) = \begin{cases} x_1 + b, & x_1 > -b, \\ 0, & x_1 \leq -b. \end{cases}$$

We define the function

$$S_s(f)(x) = \int_0^\pi \frac{|I_t f(x) - f(x)|^2}{t^{2s+1}} dt,$$

where

$$I_t f(x) = \int_{C(x,t)} f(\xi) d\xi,$$

$C(x,t) = \{\xi \in \mathbb{S}^{d-1} | \arccos(\xi \cdot x) \leq t\}$.

Here, $f_{C(x,t)} f(\xi) d\xi = |C(x,t)|^{-1} \int_{C(x,t)} f(\xi) d\xi$ is the averaged integral, where $|C(x,t)|$ is the Lebesgue measure of $C(x,t)$. Then, by [Barceló et al. 2020, Thm. 1.1], we have $f \in H^s(\mathbb{S}^{d-1})$ if and only if $S_s(f)$ is integrable. We now show that $S_s(f)$ is integrable on both $E_1 = \{x \in \mathbb{S}^{d-1} | x_1 > -b\}$ and $E_2 = \{x \in \mathbb{S}^{d-1} | x_1 < -b\}$ if $s < 3/2$. First, we define the function

$$h(x) = x_1 + b.$$

Then, $h \in H^s(\mathbb{S}^{d-1})$. If we can show that

$$S_s(h - f)(x) = \int_0^\pi \frac{|I_t (h - f)(x) - (h - f)(x)|^2}{t^{2s+1}} dt$$

is integrable on $E_1$, then we have

$$\int_{E_1} S_s(f)(x) dx = \int_{E_1} \int_0^\pi \frac{|I_t f(x) - f(x)|^2}{t^{2s+1}} dt dx
\leq 2 \int_{E_1} \int_0^\pi \frac{|I_t h(x) - h(x)|^2 + |I_t (h - f)(x) - (h - f)(x)|^2}{t^{2s+1}} dt dx
\leq 2 \int_{E_1} S_s(h)(x) dx + 2 \int_{E_1} S_s(h - f)(x) dx < \infty.$$

Assume $x \in E_1$, and let $\rho$ be the minimum angular distance between $x$ and any point in the set $S = \{\xi \in \mathbb{S}^{d-1} | \xi_1 = -b\}$, i.e., $\rho = \min_{\xi \in S} \arccos(\xi \cdot x)$. Then, for $0 < t \leq \rho$, we clearly have $I_t (h - f)(x) = 0 = (h - f)(x)$. Assume $\rho < t < \pi$. We divide $C(x, t)$ into two parts $C_1$ and $C_2$, up to a Lebesgue null set, where $C_1 = C(x,t) \cap E_1$. Then, $h - f = 0$ on $C_1$. Next, by [L 2011], we know that the measure of $C_2$ satisfies

$$\frac{|C_2|}{|C(x, t)|} = \Theta \left( I \left( \frac{t^2 - \rho^2}{t^2}; \frac{d-1}{2} \right) \right) = \Theta \left( B \left( \frac{t^2 - \rho^2}{t^2}; \frac{d}{2}; \frac{1}{2} \right) \right), \quad t \to \rho^+,$$

where $I$ is the regularized incomplete beta function and $B$ is the incomplete beta function. Here and throughout the proof, the constants in the big-$\Theta$ notations are independent of $\rho$ or $t$, but possibly depend on $b$ and $d$, which are fixed in the proof. Moreover, we have the formula

$$B \left( \frac{t^2 - \rho^2}{t^2}; \frac{d}{2}; \frac{1}{2} \right) = \frac{[(t^2 - \rho^2)/t]^d/2}{d/2} F \left( \frac{d}{2}; \frac{d+2}{2}; \frac{t^2 - \rho^2}{t^2} \right),$$

For two functions $\alpha(t)$ and $\beta(t)$, we say $\alpha(t) = \Theta(\beta(t))$ as $t \to \rho^+$ if there exist positive constants $C_1, C_2$ and radius $r > 0$ such that $C_1 \beta(t) \leq \alpha(t) \leq C_2 \beta(t)$ for all $0 < t - \rho < r$. 

\footnote{For two functions $\alpha(t)$ and $\beta(t)$, we say $\alpha(t) = \Theta(\beta(t))$ as $t \to \rho^+$ if there exist positive constants $C_1, C_2$ and radius $r > 0$ such that $C_1 \beta(t) \leq \alpha(t) \leq C_2 \beta(t)$ for all $0 < t - \rho < r$.}
where $F$ is the hypergeometric function that converges to 1 as $t \to \rho^+$ [Lozier et al., 2003, sect. 8.17, sect. 15.2]. Hence, we have

$$
\frac{|C_2|}{|C(x, t)|} = \Theta\left(\frac{(t - \rho)^{d/2}}{t^{d/2}}\right), \quad t \to \rho^+.
$$

(58)

Now, by the way we defined $h - f$, there exist constants $R_1, R_2 > 0$ such that

$$
|h - f| (\xi) \leq R_1(t - \rho), \quad \xi \in C_2,
$$

$$
|h - f| (\xi) \geq R_2(t - \rho), \quad \xi \in \bigg\{\xi \in C_2 \bigg| \min_{\theta \in S} \arccos(\xi \cdot \theta) \geq \frac{t - \rho}{2}\bigg\}.
$$

This gives us

$$
\left| \int_{C(x, t)} (h - f)(\xi)d\xi \right| = \Theta\left(\frac{(t - \rho)^{d+2}/2}{t^{d/2}}\right), \quad t \to \rho^+.
$$

(59)

Now, we have

$$
S_s(h - f)(x) = \int_0^\pi t^{-2s-1}I_2(h - f)(x)^2dt = \int_0^\pi t^{-2s-1}\left(\int_{C(x, t)} (h - f)(\xi)d\sigma(\xi)\right)^2 dt
$$

$$
= \Theta\left(\int_0^\pi t^{-2s-1-d(t - \rho)^{d+2}} dt \right) = \Theta(\rho^{2-2s} + 1).
$$

To integrate $S_s(h - f)$ over $E_1$, we first change the coordinates and integrate over $\mathbb{R}^{d-2}$ by fixing a $\rho$. The resulting integral is still in $\Theta(\rho^{2-2s} + 1)$. We then integrate over $\rho$ and the result follows from the fact that a function in $\Theta(\rho^{2-2s} + 1)$ is integrable near $\rho = 0$ if and only if $s < 3/2$. This proves $S_s(h - f)$ is integrable on $E_1$ if and only if $s < 3/2$. Note that if $S_s(h - f)$ is not integrable on $E_1$, then $S_s(f)$ is neither integrable. This proves the proposition when $s \geq 3/2$.

To see $S_s(f)$ is integrable over $E_2$ when $s < 3/2$, we note that $f$ can be rewritten as $\hat{f} - \hat{h}$, where $\hat{f}(x) = \text{ReLU}(-x_1 - b)$ and $\hat{h}(x) = -x_1 - b$. By the same argument, we have that $S_s(f) = S_s(\hat{f} - \hat{h})$ is integrable on $E_2$, which completes the proof. \hfill \Box

### E.2 Frequency biasing with a squared Sobolev norm as the loss function

In this section, we prove Theorem 4 on Sobolev training. Recall that we compute the $H^s$-based loss based on eq. (18).

**Proof of Theorem 4** Fix some $0 \leq \ell \leq L$. We can write

$$
H^\infty P_\omega y^\ell = \sum_{j=0}^{\ell_{\max}} \sum_{p=1}^{N(d, j)} H^{\infty} \omega_j a_{j, p}^\ell y^\ell = \sum_{p=1}^{N(d, \ell)} H^{\infty} \omega_{\ell, p} \hat{g}_{\ell, p} + \sum_{j=0}^{\ell_{\max}} \sum_{p=1}^{N(d, j)} H^{\infty} \omega_j a_{j, p} e_{i, j, p}^\ell,
$$

(60)

where $\omega_{\ell} = (1 + \ell)^2$ and we used the fact that

$$
a_{j, p}^\ell y^\ell = \int_{\mathbb{S}^{d-1}} Y_{j, p}(\xi) g_\ell(\xi) d\xi + e_{i, j, p}^\ell = \begin{cases} \hat{g}_{\ell, p} + e_{i, j, p}^\ell, & \text{if } \ell = j, \\ \hat{e}_{i, j, p}^\ell, & \text{otherwise}. \end{cases}
$$

Next, we have

$$
(H^{\infty} a_{j, p})_i = \int_{\mathbb{S}^{d-1}} K^{\infty}(x_i, \xi) Y_{j, p}(\xi) d\xi + e_{i, j, p}^b = \mu_j Y_{j, p}(x_i) + e_{i, j, p}^b,
$$

where the last equality follows from the Funk–Hecke formula. Hence, the first term in eq. (60) can be written as

$$
\left(\sum_{p=1}^{N(d, \ell)} H^{\infty} \omega_{\ell, p} \hat{g}_{\ell, p}\right)_i = \sum_{p=1}^{N(d, \ell)} (\mu_j Y_{\ell, p}(x_i) + e_{i, \ell, p}^b) \omega_{\ell, p} \hat{g}_{\ell, p} = \sum_{p=1}^{N(d, \ell)} e_{i, \ell, p}^b \omega_{\ell, p} \hat{g}_{\ell, p}.
$$

25
Moreover, the second term in eq. (60) can be written as
\[
\left( \sum_{j=0}^{\ell_{\text{max}}} \sum_{p=1}^{N(d,j)} H^\infty \omega_j a_{j,p} e_i^{\ell,j,p} \right)_i = \sum_{j=0}^{\ell_{\text{max}}} \sum_{p=1}^{N(d,j)} \omega_j e_i^{\ell,j,p} \left( \mu_j Y_{j,p}(x_i) + e_i^{b,j,p} \right).
\]
Therefore, we have
\[
H^\infty P_s y^\ell = \mu_\ell y^\ell + \omega_i \varepsilon^\ell_i,
\]
where
\[
(\varepsilon^\ell_i)_i = \sum_{p=1}^{N(d,\ell)} \varepsilon^\ell_i e_i^{\ell,j,p} + \sum_{j=0}^{\ell_{\text{max}}} \sum_{p=1}^{N(d,j)} \omega_j e_i^{\ell,j,p} \left( \mu_j Y_{j,p}(x_i) + e_i^{b,j,p} \right).
\]
Applying eq. (61) recursively, we have
\[
(I - 2\eta H^\infty P_s)^k y = \sum_{\ell=0}^{L} (1 - 2\eta \mu_\ell \omega_\ell)^k y^\ell - 2\eta \sum_{\ell=0}^{L} \sum_{t=0}^{k-1} (1 - 2\eta \mu_\ell \omega_\ell)^t (I - 2\eta H^\infty P_s)^{k-t-1} \omega_i \varepsilon^\ell_i.
\]
Now, since $H^\infty P_s$ is self-adjoint and positive definite in $(\mathbb{R}^n, \langle \cdot, \cdot \rangle_{P_s})$, by the way we pick $\eta$, we guarantee that $I - 2\eta H^\infty P_s$ is positive definite in $(\mathbb{R}^n, \langle \cdot, \cdot \rangle_{P_s})$ and hence
\[
\|I - 2\eta H^\infty P_s\|_{P_s} \leq 1 - 2\eta \lambda_0.
\]
This gives us $\|\varepsilon_i\|_{P_s} \leq \sum_{\ell=0}^{L} \mu_\ell^{-1} \|\varepsilon^\ell_i\|_{P_s}$, and the result follows from Theorem[1] □

While Theorem[3] captures the frequency biasing in squared $H^s$ loss training up to quadrature errors, analyzing the quadrature errors can be task-specific. Therefore, studying the quadrature rules could be a direction of future research.

F Experimental details

We now present the details of the three experiments in Section 6.

F.1 Learning trigonometric polynomials on the unit circle

In section[6] we train a NN with data derived from sampling a trigonometric polynomial at nonuniform points on the unit circle. The $n = 1140$ nonuniform data points $\{x_i\}$ for this test are generated by taking the union of three sets of equally spaced points, as shown in Figure 1. The data set $\{(\cos(\theta_i), \sin(\theta_i))\}$ contains 100 equally spaced nodes sampled from $\theta \in (0, 2\pi)$, superimposed with 40 equally spaced nodes sampled from $\theta \in [0, 0.3\pi]$ and 1000 equally spaced nodes sampled from $\theta \in [1.4\pi, 1.8\pi]$ (see Figure 1 left). We construct the quadrature weights $c_j$ by minimizing $\sum_{j=1}^{n} c_j^2$, under the constraints that the $c_i$’s are positive and the quadrature rule is exact on $\Pi_{55}^2$. Here, 55 is selected as it is close to the maximum degree such that we can efficiently solve the optimization problem for the quadrature weights.

The experiment consists of two parts. First, we compare the effects of training with the loss function $\Phi$ based on eq. (11) against the squared $L^2$ loss function $\tilde{\Phi}$ in eq. (3), where
\[
\Phi(W) = \frac{1}{2n} \sum_{i=1}^{n} |\mathcal{N}(x_i) - g(x_i)|^2, \quad \tilde{\Phi}(W) = \frac{1}{2} \sum_{i=1}^{n} c_i |\mathcal{N}(x_i) - g(x_i)|^2.
\]
We define the target function to be
\[
g(x) = g(\theta) = \sum_{\ell=1}^{9} \sin(\ell \theta), \quad x = x(\theta) = (\cos \theta, \sin \theta) \in \mathbb{S}^1,
\]
where $g(\theta) = g(\theta(x))$. We set up two 2-layer ReLU-activated NNs with $5 \times 10^4$ hidden neurons in each layer and train them using the same training data and gradient descent procedure, except with different loss functions $\Phi$ and $\tilde{\Phi}$. 

26
We set \( \ell \) the squared Sobolev norm as the loss function (see eq. (18)). In addition, we also train the NN to learn each individual frequency with the training data coming from \( g_{\ell} = \sin(\ell \theta) \) and count the number of iterations it takes to obtain \( \Phi(W) < 1.0 \times 10^{-3} \) (see Figure 1, right).

The second part of the experiment focuses on NN training with a discretized squared Sobolev norm as the loss function. More precisely, we fix some \( s \in \mathbb{R} \) and consider the Sobolev loss function eq. (18). For \( S^1 \), we have \( N(d, \ell) = 2 \) if \( \ell > 0 \). We take \( Y_{\ell,1}(x) = \sin(\ell \theta) / \sqrt{2\pi} \) and \( Y_{\ell,2}(x) = \cos(\ell \theta) / \sqrt{2\pi} \), where the \( \sqrt{2\pi} \) factor is a normalization factor.

We set \( \ell_{\text{max}} = 30 \) in eq. (18) and learn \( g \) with different \( s \) values ranging from \(-1\) to \(4\). For each \( s \), we compute the frequency loss \( |\hat{N}(\ell) - \hat{g}(\ell)| \) after different numbers of epochs. As \( s \) increases, the frequency loss for higher frequencies decays faster (see Figure 2). In particular, we see in Figure 2 the “rainbow” plot, that when \( s = -1 \), the lower-frequency losses are much smaller than the higher ones after 5000 iterations, while when \( s = 3 \) the higher frequencies are learned faster than the lower ones.

F.2 Learning spherical harmonics on the unit sphere

In section 6.2 we train a NN with data derived from sampling function defined on \( S^2 \) at nonuniform points. The training data is a maximum determinate set of 2500 points that comes from the so-called “sphrepts” dataset [Wright and Michaels, 2015]. In this experiment, the target function is

\[
g(x) = \sum_{\ell=1}^{15} Y_{2\ell,0}(x),
\]

where \( Y_{2\ell,0} \) is the normalized zonal spherical harmonic function of degree \( 2\ell \). Therefore, the spherical harmonic coefficients of \( g \) defined in eq. (4) satisfy \( \hat{g}_{\ell,p} = 1 \) if \( p = 0 \) and \( \ell = 2, 4, \ldots, 30 \), and \( \hat{g}_{\ell,p} = 0 \) otherwise. We then train an NN with the squared \( H^s \) norm as the loss function (see eq. (18)) for \( s = -1, 0, 2.5 \). By Theorem 4, we need \( \ell_{\text{max}} \geq L = 30 \). We set \( \ell_{\text{max}} = 40 \) in eq. (18), assuming that the bandwidth \( L \) is not known a priori. We observe frequency biasing in this experiment by considering \( |\hat{N}_{\ell,p} - \hat{g}_{\ell,p}| \) after each epoch for \( \ell = 4, 10, 20 \). We confirm that low frequencies of \( g \) are captured earlier in training than high frequencies when \( s = -1 \) and \( s = 0 \) (see Figure 3, left and middle), and that this frequency biasing phenomena can be counterbalanced by taking \( s = 2.5 \) (see Figure 3, right).
F.3 Test on Autoencoder

Autoencoders can be used as a generative models to randomly generate new data that is similar to the training data. In this experiment, we use Sobolev-based norms to improve NN training for producing new images of digits that match the MNIST dataset. In our final experiment, we use the same autoencoder architecture as in Chollet [2016], except with the loss function (64), for s = -1, 0, 1. We first pollute the training images with low-frequency noise and train the NN, hoping that the trained NN will act as filter for the noise. We see that training the NN with eq. (65) for s = 1 gives us the best results due to the high-frequency biasing induced by the choice of the loss function. Although \( \mathbf{H}^\infty \) is low frequency biasing, the high-frequency biasing of...
$J_s^\top J_s$ dominates for sufficiently large $s$. In that case, the low-frequency noise barely changes the training in the earlier epochs as the low-frequency components of the residual correspond to small eigenvalues of $H^\infty (I \otimes J_s^\top J_s)$. Similar results are discussed in Engquist et al. [2020] and Zhu et al. [2021] in the inverse problem and image processing contexts, respectively.

The opposite phenomenon occurs when we add high-frequency noise (see Figure 4, bottom row). Since $H^\infty$ by itself makes the NN training procedure bias towards low-frequencies, the output for $s = 0$ does already filter high-frequency noise. Since $J_s^\top J_s$ for $s < 0$ further biases towards low-frequencies, one can obtain better high-frequency filters. We observe that the best denoising results for the autoencoder comes from selecting $s = -1$ (see Figure 4, bottom row).