SMALLER GENERALIZATION ERROR DERIVED FOR DEEP COMPARED TO SHALLOW RESIDUAL NEURAL NETWORKS

AKU KAMMONEN, JONAS KIESSLING, PETR PLECHÁČ, MATTIAS SANDBERG, ANDERS SZEPESSY, AND RAÚL TEMPONE

Abstract. Estimates of the generalization error are proved for a residual neural network with \( L \) random Fourier features layers \( \tilde{z}_{\ell+1} = \tilde{z}_\ell + \text{Re} \sum_{k=1}^{K} b_{\ell k} e^{i\omega_{\ell k} \tilde{z}_\ell} + \text{Re} \sum_{k=1}^{K} c_{\ell k} e^{i\omega'_{\ell k} \cdot x} \). An optimal distribution for the frequencies \((\omega_{\ell k}, \omega'_{\ell k})\) of the random Fourier features \( e^{i\omega_{\ell k} \tilde{z}_\ell} \) and \( e^{i\omega'_{\ell k} \cdot x} \) is derived. The derivation is based on the corresponding generalization error to approximate function values \( f(x) \). The generalization error turns out to be smaller than the estimate \( \| \hat{f} \|_{L^1(R^d)} / (LK) \) of the generalization error for random Fourier features with one hidden layer and the same total number of nodes \( LK \), in the case the \( L^\infty \)-norm of \( f \) is much less than the \( L^1 \)-norm of its Fourier transform \( \hat{f} \). This understanding of an optimal distribution for random features is used to construct a new training method for a deep residual network that shows promising results.

Keywords. residual network, deep random feature, supervised learning, error estimates, layer by layer algorithm.

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1. Introduction

1.1. Residual neural network formulation. We study approximation properties of deep residual neural networks applied to the supervised learning with a given data set \( \{(x_n, y_n) \in \mathbb{R}^d \times \mathbb{R} | n = 1, \ldots, N \} \), where the \( x_n \) are independent samples from an unknown probability distribution. We consider the noisy data \( y_n = f(x_n) + \epsilon_n \), for some function \( f: \mathbb{R}^d \to \mathbb{R} \), with its Fourier transform bounded in \( L^1(\mathbb{R}^d) \). The noise \( \{\epsilon_n\}_{n=1}^N \) are independent random variables, also independent of the data \( \{x_n\}_{n=1}^N \), with the second moment \( \epsilon^2 = \mathbb{E}[\epsilon_n^2] \). The objective is to use the data in order to determine a neural network approximation that approximates the function \( f \) as accurately as possible.

We focus on a particular case of a residual neural network with the network activation function \( s(\omega, x) = e^{i\omega \cdot x} \). We denote \( \omega \cdot x = \sum_{i=1}^d \omega^i x^i \) the standard Euclidean product on \( \mathbb{R}^d \). In effect we construct a multi-layer (deep) random Fourier feature approximation.

To motivate the use of the random Fourier features in the presented analysis we first introduce a neural network with a single hidden layer with \( K' \) nodes and the activation function \( s(\omega, x) = e^{i\omega \cdot x} \). The related standard neural network approximation problem, cf. [13], requires to find the amplitudes \( \tilde{c}_k \in \mathbb{C} \) and frequencies \( \omega'_k \in \mathbb{R}^d, k = 1, \ldots, K' \), which minimize the risk functional, i.e., solving the problem

\[
\min_{(\omega_k, \tilde{c}_k) \in \mathbb{R}^d \times \mathbb{C}} \sum_{n=1}^N \left| y_n - \text{Re} \sum_{k=1}^{K'} \tilde{c}_k e^{i\omega'_k \cdot x_n} \right|^2
\]
which for \( N \to \infty \) becomes the generalization error

\[
\min_{(\omega_k, \bar{c}_k) \in \mathbb{R}^d \times \mathbb{C}} \mathbb{E}_{xy}[|y - \text{Re} \sum_{k=1}^{K'} \bar{c}_k e^{i \omega_k \cdot x}|^2].
\]

We shall denote the expected value with respect to the data distribution by \( \mathbb{E}_{xy} \) and the expected value with respect to the distribution of frequencies by \( \mathbb{E}_{\omega} \).

Here we relax problem (1.1) by studying a more tractable problem, namely we assume instead that the frequencies \( \{\omega_k \in \mathbb{R}^d \mid k = 1, \ldots, K'\} \) are independent, identically distributed (iid) random variables with a certain distribution \( \bar{p}' : \mathbb{R}^d \to [0, \infty) \). Then the generalization error for a random Fourier feature neural network with one hidden layer and \( K' \) nodes has the bound

\[
\mathbb{E}_{\omega}[\min_{\bar{c} \in \mathbb{C}^{K'}} \mathbb{E}_{xy}[|y - \text{Re} \sum_{k=1}^{K'} \bar{c}_k e^{i \omega_k \cdot x}|^2]] \leq \frac{1}{K'} \int_{\mathbb{R}^d} |\hat{f}(\omega)|^2 \bar{p}'(\omega) \, d\omega,
\]

where we introduce the Fourier transform

\[
\hat{f}(\omega) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} f(x) e^{-i \omega \cdot x} \, dx
\]

and its inverse representation

\[
f(x) = \int_{\mathbb{R}^d} \hat{f}(\omega) e^{i \omega \cdot x} \, dx.
\]

The form (1.3) of the Fourier transform is convenient for presenting various formulas without \( 2\pi \) factors. The well known proof of (1.2), cf. [3], is based on Monte Carlo quadrature of this inverse Fourier representation, see Lemma 3.1.

The estimate (1.2) indicates the possibility to improve the bound by approximating the minimizing density \( p' = |\hat{f}|/\|\hat{f}\|_{L^1(\mathbb{R}^d)} \) (cf. Lemma 3.2) for instance by the adaptive Metropolis method in [8]. Since a minimum is less than or equal to its corresponding mean, (1.2) implies

\[
\min_{(\bar{c}_k, \omega_k) \in \mathbb{C} \times \mathbb{R}^d} \mathbb{E}_{xy}[|y - \text{Re} \sum_{k=1}^{K'} \bar{c}_k e^{i \omega_k \cdot x}|^2] \leq \mathbb{E}_{\omega}[\mathbb{E}_{xy}[|y - \text{Re} \sum_{k=1}^{K'} \bar{c}_k e^{i \omega_k \cdot x}|^2]]
\]

\[
\leq \frac{1}{K'} \int_{\mathbb{R}^d} |\hat{f}(\omega)|^2 \bar{p}'(\omega) \, d\omega,
\]

which provides an error estimate also for convergent gradient or stochastic gradient approximations of the optimization problem in the left hand side.

The aim of this work is to generalize random Fourier features to include several hidden layers and study the corresponding generalization error. In particular we prove in Theorem 2.1 that the generalization error for a deep residual neural network can be smaller than the bound (1.2) for neural networks with one hidden layer and the same number of nodes. This approximation result also shows an optimal parameter distribution, which we use to formulate a generalization of the adaptive Metropolis method [8] to deep random features networks.
We study deep residual neural networks, with \( L \) layers and \( K \) nodes per layer. We define the single layer neural network function at the layer \( \ell = 0 \)

\[
\beta(x) := \text{Re} \sum_{k=1}^{K} \bar{c}_{0k} e^{i \omega_{0k} \cdot x},
\]

and represent residuals at subsequent layers by

\[
\bar{z}_{\ell+1} = \bar{z}_{\ell} + \text{Re} \sum_{k=1}^{K} \bar{b}_{\ell k} e^{i \omega_{\ell k} \cdot \bar{z}_{\ell}} + \text{Re} \sum_{k=1}^{K} \bar{c}_{\ell k} e^{i \omega'_{\ell k} \cdot x}, \quad \ell = 1, \ldots, L - 1.
\]

The residual neural network is thus defined by the parameters \( \theta_{\ell k} = (\bar{b}_{\ell k}, \omega_{\ell k}), \theta'_{\ell k} = (\bar{c}_{\ell k}, \omega'_{\ell k}) \), \( \ell = 0, \ldots, L - 1, k = 1, \ldots, K \) that minimize the generalization error

\[
\min_{\theta_{\ell k}, \theta'_{\ell k}} \mathbb{E}_{xy} \left[ |y - \text{Re} \sum_{k=1}^{K} \bar{c}_{0k} e^{i \omega_{0k} \cdot x}|^2 \right], \quad \text{and}
\]

\[
\min_{\theta_{\ell k}, \theta'_{\ell k}} \mathbb{E}_{xy} \left[ |\bar{z}_{L} - (y - \beta(x))|^2 + \delta L \sum_{\ell=1}^{L-1} |\bar{z}_{\ell+1} - \bar{z}_{\ell}|^2 \right],
\]

subject for \( \ell = 1, \ldots, L - 1 \) to

\[
\bar{z}_{\ell+1} = \bar{z}_{\ell} + \text{Re} \sum_{k=1}^{K} \bar{b}_{\ell k} e^{i \omega_{\ell k} \bar{z}_{\ell}} + \text{Re} \sum_{k=1}^{K} \bar{c}_{\ell k} e^{i \omega'_{\ell k} \cdot x},
\]

\[
\bar{z}_{1} = 0.
\]

The final approximation then becomes (with the * indicating that the optimal parameters \( \theta_{\ell k}, \theta'_{\ell k} \) are used)

\[
f^*_L(x) := \bar{z}_L^* + \text{Re} \sum_{k=1}^{K} \bar{c}_{0k}^* e^{i \omega_{0k}^* \cdot x}.
\]

Rather than solving the non-convex minimization problem (1.7) we follow the strategy motivated by the single layer case explained above. We use random Fourier features, i.e., choosing random frequencies \( \omega_{\ell k}, \omega'_{\ell k} \) and solving first the convex minimization problem for the parameters \( \bar{c}_{0k} \)

\[
\min_{\bar{c}_{0k}} \mathbb{E}_{xy} [|y - \text{Re} \sum_{k=1}^{K} \bar{c}_{0k} e^{i \omega_{0k} \cdot x}|^2],
\]

with the solution \( \bar{c}_{0k}^*, k = 1, \ldots, K \) of (1.8) defining the single layer approximation

\[
\beta^*(x) = \text{Re} \sum_{k=1}^{K} \bar{c}_{0k}^* e^{i \omega_{0k}^* \cdot x},
\]
which in turn defines the optimization problem for the deep residual network, i.e., for 
\((b_{\ell k}, c_{\ell k}), \ell = 1, \ldots, L - 1\)

\[
\min_{(b_{\ell k}, c_{\ell k}) \in \mathbb{C} \times \mathbb{C}} \mathbb{E}_{x y} \left[ |\bar{z}_L - (y - \beta^\ast(x))|^2 + \delta L \sum_{\ell=1}^{L-1} |\bar{z}_{\ell+1} - \bar{z}_\ell|^2 \right],
\]

(1.10)

subject, for \(\ell = 1, \ldots, L - 1\), to

\[
\bar{z}_{\ell+1} = \bar{z}_\ell + \text{Re} \sum_{k=1}^{K} \bar{b}_{\ell k} e^{i \omega_{\ell k} \bar{z}_\ell} + \text{Re} \sum_{k=1}^{K} \bar{c}_{\ell k} e^{i \omega_{\ell k}^\prime x},
\]

\[
\bar{z}_1 = 0.
\]

The purpose of the initial optimization (1.8) is to obtain an optimization problem for \(\bar{z}_\ell\) with smaller data \(y - \beta^\ast(x)\) instead of \(y\), which turns out to be useful in our proof and experiments. The non negative number \(\delta\) is a regularization parameter. We include the penalty term, \(\delta L \sum_{\ell=0}^{L-1} |\bar{z}_{\ell+1} - \bar{z}_\ell|^2\), since the penalty has a role in finding an optimal solution as described in Section [4]. The random frequencies \(\omega_{\ell k}, \omega_{\ell k}^\prime\) are independent identically distributed random variables for \(\ell = 0, \ldots, L - 1\) and \(k = 1, \ldots, K\) and they are sampled from yet to be determined distributions depending on frequencies and layers.

In the case that all \(\bar{b}_{\ell k} = 0\), the formulation (1.10) is equivalent to approximation with a random Fourier feature network with one hidden layer and \(LK\) nodes. The purpose of the presented analysis is to derive estimates of the generalization error for (1.10) that improves the bound (1.2), with \(K' = LK\), and determine optimal choices of \(L, K, \bar{p}, \bar{p}', \delta\) that minimize the generalization error for (1.10).

Our analysis is based on viewing the optimization problem (1.10) as a discrete version of a continuous time optimal control problem. More precisely, in our analysis we use the solution to an optimal control problem related to (1.10) with infinite number of nodes and layers. Details of the analysis and the complete proof are in Section [4] and Section [5]. Here we outline only a basic connection between the optimization problem (1.10), viewed as a discrete optimal control, and its continuum time counter part. We postpone the detailed discussion to Section [4].

For the sake of simplicity we assume here in the introduction the data is noiseless, i.e., \(\epsilon = 0, \ y_n = f(x_n)\) for some (unknown) function \(f\). We introduce time dependent controls \(\hat{b} : [0, 1] \times \mathbb{R} \to \mathbb{C}\) and \(\hat{c} : [0, 1] \times \mathbb{R}^d \to \mathbb{R}\). We define the control function \(\alpha : [0, 1] \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}\)

\[
\alpha(t, z; x) := \text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i \omega z_t} d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega') e^{i \omega' x_t} d\omega',
\]

(1.11)

and formulate the optimal control problem with the time dependent state function \(z_t(x)\) with its dynamics defined by \(\alpha(t, z_t; x)\). Thus we solve the optimal control problem

\[
\min_{\hat{b} : [0, 1] \times \mathbb{R} \to \mathbb{C}} \min_{\hat{c} : [0, 1] \times \mathbb{R}^d \to \mathbb{C}} \mathbb{E}_x \left[ |z_1 - (f(x) - \beta(x))|^2 + \delta \int_0^1 |\alpha(t, z_t, x)|^2 dt \right],
\]

(1.12)

subject to \(\frac{dz_t}{dt} = \alpha(t, z_t; x)\)

\[
z_0 = 0.
\]
where $\beta(x)$ is defined by (1.3). The optimal control problem (1.12) can be solved explicitly as described in Lemma 4.1. This explicit solution is then used to derive the bounds (2.2) and (2.3) in Theorem 2.1, see Section 4.

The relation to the optimization problem (1.10) is obtained by using Monte Carlo approximation of integrals over $\omega$, $\omega'$ and $t$, thus introducing random times and frequencies $(t_{\ell k}, \omega_{\ell k}) \sim p(t, \omega)dt \, d\omega$, $(t'_{\ell k}, \omega'_{\ell k}) \sim p'(t', \omega')dt' \, d\omega'$ in

$$
\alpha(t, z_t; x) = \text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_t} \, d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega') e^{i\omega' x} \, d\omega',
$$

which gives the Monte Carlo approximations

$$(1.13) \quad \sum_{\ell=0}^{L-1} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_t} \, d\omega \approx \frac{1}{LK} \sum_{\ell=0}^{L-1} \sum_{k=1}^K \frac{\hat{b}(t_{\ell k}, \omega_{\ell k}) e^{i\omega_{\ell k} z_\ell}}{p(t_{\ell k}, \omega_{\ell k})},$$

$$(1.14) \quad \sum_{\ell=0}^{L-1} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}^d} \hat{c}(t, \omega') e^{i\omega' x} \, d\omega' \approx \frac{1}{LK} \sum_{\ell=0}^{L-1} \sum_{k=1}^K \frac{\hat{c}(t'_{\ell k}, \omega'_{\ell k}) e^{i\omega'_{\ell k} x}}{p'(t'_{\ell k}, \omega'_{\ell k})},$$

with $\tilde{z}_\ell := \tilde{z}(t_\ell)$ denoting the state dynamics $z_t$ evaluated at times $t_\ell = Q^{-1}(\ell)$, where $Q : [0,1] \rightarrow [0,1]$ is the cumulative distribution function for a given density $q : [0,1] \rightarrow [0,\infty)$. The random times and random frequencies are independent, therefore the distributions take the form $p(t, \omega) = \tilde{p}(\omega)q(t)$ and $p'(t', \omega') = \tilde{p}'(\omega')q'(t')$, $t_\ell = Q^{-1}(\ell)$. Thus, heuristically, in the limit $L \rightarrow \infty$ and $K \rightarrow \infty$

$$\tilde{b}_{\ell k} \approx \frac{1}{LK} \hat{b}(t_{\ell k}, \omega_{\ell k}) \quad \text{and} \quad \tilde{c}_{\ell k} \approx \frac{1}{LK} \hat{c}(t'_{\ell k}, \omega'_{\ell k}),$$

and the optimal solution of the problem (1.10) can be linked to the approximation of the optimal control solution of (1.12). The presented analysis in Section 4 clarifies this connection rigorously and a precise formulation of $t_{\ell k}, t'_{\ell k}, \omega_{\ell k}, \omega'_{\ell k}$, including stratified sampling for $t_{\ell k}, t'_{\ell k}$ related to the layers, is in Section 2.

**Remark 1.1.** The optimization problem (1.10) can be generalized to use $d$-dimensional control functions $\tilde{z}_\ell \in \mathbb{R}^d$ in which case we have $(b_{\ell k}, c_{\ell k}) \in \mathbb{C}^d \times \mathbb{C}^d$. For a given, fixed vector $e \in \mathbb{R}^d$ we then have an optimization problem analogous to (1.10)

$$\min_{(b_{\ell k}, c_{\ell k}) \in \mathbb{C}^d \times \mathbb{C}^d} \mathbb{E}_{xy} \left[ |e \cdot \tilde{z}_L - (y - \beta(x))|^2 + \delta L \sum_{\ell=0}^{L-1} |\tilde{z}_{\ell+1} - \tilde{z}_\ell|^2 \right],$$

subject, for $\ell = 1, \ldots, L - 1$, to

$$(1.15) \quad \tilde{z}_{\ell+1} = \tilde{z}_\ell + \text{Re} \sum_{k=1}^K \bar{b}_{\ell k} e^{i\omega_{\ell k} z_\ell} + \text{Re} \sum_{k=1}^K \bar{c}_{\ell k} e^{i\omega'_{\ell k} x},$$

$$\tilde{z}_1 = 0,$$

with a similar error estimate as for (1.10). A common formulation is to let all $\tilde{c}_{\ell k} = 0$, see [4] where also a different regularization term is used. Then the initial data is typically $\tilde{z}_0 = x$ instead of $\tilde{z}_0 = 0$. The vector $e$ can also be replaced by another vector and the dimension of the vectors could be different from $d$.

**Remark 1.2.** The derivation of the error estimates here shows an advantage to include non zero coefficients $\bar{c}_{\ell k}$, which also can be motivated from the perspective to use a Markov
control allowed to depend on both the state $z_\ell$ and the data $x$. The inclusion of such previous layers in the dynamics of the state in deep neural networks is studied in so called deep dense neural networks, see [7]. Note that the control variables $\bar{b}_\ell k$ and $\bar{c}_\ell k$ only depend on the distribution of the data $\{(x_n, y_n) \mid n = \mathbb{Z}_+\}$ and not on the individual outcomes.

1.2. Relation to previous work. The main inspiration of our work is the construction and optimal control analysis of deep residual neural networks in [5], which proves an error estimate of the generalization error including also the more demanding case with finite sets of data $(x, y)$. That error estimate does not improve the error estimate compared to approximation with a single hidden layer. Other important previous results are the formulation of random Fourier features in [10] and the optimal control perspective in [4]. The main new mathematical idea in our work is to identify a simple structure in a related infinite dimensional optimal control problem (1.12) and use it to identify the partition of the control into two parts: one part depending on the data $x$ and another part depending on the state $z_\ell$; and then use the two parts to minimize the variance of the Monte Carlo quadrature present in deep residual neural networks. The mathematical technique used in our work is a combination of standard Monte Carlo approximations adapted to the error analysis of approximations of differential equations and optimal control problems, where the approximation error is represented as an integral of the difference of the exact and approximate value functions along the exact solution path, as e.g., in [14].

There are several results on improved approximation for deep neural networks as compared to shallow networks for certain functions, e.g., in [15], [11], [12]. The work [11] proves that also the generalization error obtained from the stochastic gradient method can be smaller for three layer neural networks, based on a residual neural network of the form (1.10), compared to kernel methods using the same number of stochastic gradient descent steps. The result uses the rectifier linear unit activation function, $v \mapsto \max(0, v)$, instead of the Fourier activation function $v \mapsto e^{iv}$ used here. The example providing better approximation in neural networks with three layers are based on composition functions related to the neural network construction.

Our Theorem 2.1 also estimates the generalization error instead of the minimal error in a certain norm, as in [15], [11], [12]. The error estimate in Theorem 2.1 is not based on functions related to the compositions given by the neural network, as in [11], instead on functions with $L^1$-bounded Fourier transform. The theorem establishes insight on the optimal distribution of all parameters for the deep residual network (1.10). The theorem also shows that for some functions $f$, with $\|f\|_{L^\infty(\mathbb{R}^d)} \ll \|\hat{f}\|_{L^1(\mathbb{R}^d)}$, supervised learning with deep networks could have less generalization error compared to networks with one hidden layer. Note that we study upper bounds here, so we cannot conclude that deep residual networks have smaller generalization errors than shallow: although the Monte Carlo approximation error we use is sharp, the minimization error can be smaller depending on the regularity of the $x$ sampling density, see [2]. Clearly other deep neural networks could have better approximation by other reason as those studied here. The purpose of studying the special network (1.10) is that for this particular setting we can provide theoretical motivation on the approximation and its optimal distribution of parameters.

We present the result in Section 2 and split the proof together with the computational demonstration in the subsequent five sections. Section 3 provides background on Monte Carlo quadrature and Section 4 presents the optimal control solution of the related problem
to (1.10) with infinite number of layers $L$ and nodes per layer $K$. The lemmas in these two sections are then used in Section 5 which proves the main result in Theorem 2.1. Sections 6 and 7 present new numerical algorithms and experiments, using the obtained optimal random feature distribution, to approximate the deep residual network problem (1.10) based on finite amount of data and adaptive Metropolis sampling of the frequencies. In particular numerical tests confirm that deep residual networks can have smaller generalization error compared to networks with one hidden layer and the same total number of nodes. The final Section 8 includes a short summary of the work.

2. Statement and discussion of the main result

We begin with stating the main result and present the proof and supporting lemmas in subsequent sections. The result provides the optimal densities $p(t, \omega) dt d\omega$, $p(t', \omega') dt' d\omega'$ and sharp upper bounds on the generalization error of the studied residual neural network. The use of the optimal densities in time-frequency domains for Monte Carlo approximation of integrals is one of the principal features, thus we first explain the construction of the Monte Carlo approximation based on a stratified sampling approach.

To each random frequency $\omega_{\ell k}$ we associate a random time $t_{\ell k} \in [0, 1]$ with the purpose to construct Monte Carlo approximations of the integrals over $\mathbb{R}^d \times [0, 1]$ in (1.13), such that each layer $\ell$ has $K$ independent times $t_{\ell k}$, $k = 1, \ldots, K$, where $K$ is fixed and non random. While the sampling of random frequencies $\omega_{\ell k}$ and $\omega'_{\ell k}$ is straightforward, for the random times $t_{\ell k}$ and $t'_{\ell k}$ we employ stratified sampling as follows. For a given density $q : [0, 1] \to [0, \infty)$ we denote its cumulative distribution function $Q(t) := \int_0^t q(s) ds$. Then, for each layer $\ell \in \{0, \ldots, L-1\}$ let $\tau_{\ell k}$, $k = 1, \ldots, K$ be independent and uniformly distributed random variables on $[\ell L, (\ell + 1)L)$, independent also of all $\omega_{\ell k}$ and all $\omega'_{\ell k}$. We define the random times $t_{\ell k} := Q^{-1}(\tau_{\ell k})$ and the non-random time levels $t_\ell := Q^{-1}(\frac{\ell}{L})$, see Figure 1. Assuming that $t \in [t_\ell, t_{\ell+1})$ then the density for the random variable $t_{\ell k}$ is given by

$$
P(t_{\ell k} \in [t, t + dt)) = \mathbb{P}(\tau_{\ell k} \in [Q(t), Q(t + dt)]) = \frac{q(t)dt}{L^{-1}} = Lq(t)dt.$$ 

We also define the space time density $p(t, \omega) := \bar{p}(\omega)q(t)$. Similarly we associate $t'_{\ell k}$ with the density $q' : [0, 1] \to [0, \infty)$ to $\omega_{\ell k}$ and define $p'(t, \omega) := \bar{p}'(\omega)q'(t)$.

In order to state the result with rigorous technical assumptions we select $h : \mathbb{R} \to \mathbb{R}$ to be a Schwartz function which is equal to one on $[-1, 1]$, for example,

$$h(z) = \begin{cases} 
(1 + e^{\frac{1}{1-z^2}}) e^{-(1-z)^2} & \text{for } z > 1, \\
1 & \text{for } |z| \leq 1, \\
(1 + e^{\frac{1}{1+z^2}}) e^{-(1+z)^2} & \text{for } z < -1.
\end{cases}$$
Figure 1. Stratified sampling of \( t_{\ell_k} \) with four layers and the density proportional to \( q \). The red curve is the graph \( Q : [0, 1] \to [0, 1] \).

Theorem 2.1. Assume that the quantities

\[
F := \|f\|_{L^\infty(\mathbb{R}^d)} , \\
A := \int_{\mathbb{R}^d} \frac{|\hat{f}(\omega)|^2}{\tilde{p}'(\omega)} \, d\omega , \\
B' := F^2 \int_{\mathbb{R}} \frac{|\partial_\omega \hat{h}(F\omega)|^2}{\tilde{p}(\omega)} \, d\omega , \\
B := B' \exp \left( 2\|\partial_z(zh(z/F))\|_{L^\infty(\mathbb{R})} \right) , \\
F\|\omega \partial_\omega \hat{h}(F\omega)\|_{L^2(\mathbb{R})} + \frac{\|F\partial_\omega \hat{h}(F\omega)\|^2}{\tilde{p}(\omega)} \|_{L^\infty(\mathbb{R})} + \|\partial_z^2(zh(z/F))\|_{L^\infty(\mathbb{R})} + \|\hat{f}\|_{L^\infty(\mathbb{R}^d)} ,
\]

are bounded and \( \bar{z}^* \) is an optimal solution to \([1.10]\) and \( \beta^*(x) \) an optimal solution to \([1.8]\), then there are positive constants \( c \) and \( C \) such that the generalization error satisfies

\[
(2.1) \quad \mathbb{E}_{t_\omega}[\mathbb{E}_{x,y}[|\bar{z}^*_L + \beta^*(x) - y|^2]] \leq \frac{C}{LK} + \mathcal{O} \left( \frac{1}{K^2} + \frac{1}{L^4} + Le^{-cK} + \frac{\epsilon}{\sqrt{LK}} + \epsilon^2 + \delta \right).
\]

Furthermore, the minimal value of the constant \( C \) given by

\[
(2.2) \quad C = B^2(1 + \log \frac{A^*}{B^*})^2 ,
\]
is obtained for the optimal time dependent densities,
\[
p'(t, \omega) = \bar{p}'(\omega) q'(t) = \begin{cases} \frac{|\hat{f}(\omega)|}{\|f\|_{L^1([0,1])}} & t < t_* := \min(1, \frac{B_*}{A_*}), \\
0 & t \geq t_*, \end{cases}
\]
(2.3)
\[
p(t, \omega) = \bar{p}(\omega) q(t) = \begin{cases} \frac{t^{-1}|\partial_\omega \hat{h}(F\omega)|}{\|t^{-1}|\partial_\omega \hat{h}(F\cdot)|\|_{L^1([t_*,1])}} & t < t_*, \\
0 & t \geq t_*, \end{cases}
\]
\[
A_* := \|\hat{f}\|_{L^1(\mathbb{R}^d)},
B_* := \|\partial_\omega \hat{h}(F\cdot)\|_{L^1(\mathbb{R})} \exp \left( \|\partial_x (zh(z/F))\|_{L^\infty(\mathbb{R})} \right),
\]
while if \(q\) and \(q'\) are constant the minimal constant is
\[
C = \min \left( 2(AB)^{1/2} - B, A \right).
\]

We note that if \(\frac{B_*}{A_*}\) is sufficiently small then \(C \ll A_*^2\). We have for a positive constant \(c\) that \(A_* = \|\hat{f}\|_{L^1(\mathbb{R}^d)}\) and \(B_* = \mathcal{O}(\|f\|_{L^\infty(\mathbb{R})}e^{c\|f\|_{L^\infty(\mathbb{R})}})\). For instance a regularized discontinuity as \(f(x) = e^{-|x|^2/2} \int_0^{x/a} \sin t \, dt\) has \(\|f\|_{L^\infty(\mathbb{R})} \ll \|\hat{f}\|_{L^1(\mathbb{R})}\) for \(0 < a \ll 1\). Therefore there are functions \(f\) such that the deep dense residual neural networks (1.10) and (1.15) have a more accurate estimate (2.1) as compared to the estimate (1.2) for the corresponding neural network with one hidden layer. We note in the case that \(\frac{B_*}{A_*}\) is sufficiently small then \(C \simeq 2(AB)^{1/2} \ll A\). The optimal densities \(\bar{p}'\) and \(\bar{p}\) that minimize \(A\) and \(B'\), respectively, for time independent densities are
\[
A = \|\hat{f}\|_{L^1(\mathbb{R}^d)}^2 \text{ for } \bar{p}'(\omega) = \frac{|\hat{f}(\omega)|}{\|\hat{f}\|_{L^1(\mathbb{R}^d)}},
\]
(5.5)
\[
B' = \|\partial_\omega \hat{h}(F\omega)\|_{L^1(\mathbb{R})}^2 \text{ for } \bar{p}(\omega) = \frac{|\partial_\omega \hat{h}(F\omega)|}{\|\partial_\omega \hat{h}(F\cdot)\|_{L^1(\mathbb{R})}},
\]
as shown in Lemma 3.2. The optimal time-dependent densities are derived in Lemma 4.2. The error term \(\frac{C}{LK}\) in (2.1) dominates provided
\[
L \ll K \ll L^3,
\]
\[
\tilde{\delta} + \epsilon^2 \ll (LK)^{-1}.
\]

Analogous to the estimate (1.4) for one hidden layer, we obtain by Theorem 2.1 a bound on the approximation error for the following minimization problem.

**Corollary 2.2.** Suppose the assumptions in Theorem 2.1 hold, then the generalization error has the bound
\[
\min_{(\omega_k, \omega_0) \in \mathbb{R} \times \mathbb{R}^d} \mathbb{E}_{x,y} [\|\bar{z}_L^* + \beta(x) - y\|^2] \leq \frac{C}{LK} + \mathcal{O}\left( \frac{1}{K^2} + \frac{1}{L^4} + \tilde{\delta} + L e^{-cK} + \epsilon^2 + \frac{\epsilon}{(LK)^{1/2}} \right)
\]
where \(C\) satisfies (2.2).

The main idea in the proof is to use a Monte Carlo approximation of the corresponding optimal control problem with infinite number of layers \(L\) and nodes \(K\). The problem with infinite number of nodes is solved explicitly in Section 4 and shows that the state, corresponding to \(\bar{z}_k\), for each data point \(x\) is a linear function in the levels from the initial state to
the final state $y(x)$. This simple linear dependence makes it possible to split the Monte Carlo approximation

$$
\text{Re} \sum_{k=1}^{K} \bar{b}_k e^{i \omega_k \cdot x} + \text{Re} \sum_{k=1}^{K} \bar{c}_k e^{i \omega_k \cdot x},
$$

where the first term approximates a scaled identity map and the second term approximates the data $y(x)$. The variances of these two Monte Carlo approximations are optimized by the sampling densities (2.3) and yield smaller error than the one hidden layer estimate (1.2) in the case $\|f\|_{L^\infty(\mathbb{R}^d)} \ll \|\hat{f}\|_{L^1(\mathbb{R}^d)}$.

To use the approximation result of the theorem in practise requires to sample from the optimal densities. In Section 6 we present an explicit layer by layer approximation of (1.10) combined with an adaptive Metropolis method that approximately samples the frequencies optimally, following [8].

### 3. Random feature Monte Carlo approximation

The proof of Theorem 2.1 is based on Monte Carlo approximation of a solution to an optimal control problem with infinite number of layers and nodes. The basic case of approximation with one hidden layer is studied in this section.

If we set $\bar{b}_k = 0$ in (1.10) or (1.15) we obtain a random Fourier feature network with one hidden layer

$$
\min_{\bar{c}_{\ell k} \in \mathbb{C}} \mathbb{E}_{x,y}[|\bar{z}_L - (y - \beta(x))|^2],
$$

subject to

$$
\bar{z}_L = \text{Re} \sum_{\ell=1}^{L-1} \sum_{k=1}^{K} \bar{c}_{\ell k} e^{i \omega_k \cdot x}.
$$

The generalization error (1.2) and the optimal choice of the density, namely $\bar{p}' = |\hat{f}|/\|\hat{f}\|_{L^1(\mathbb{R}^d)}$ in (2.5), follows by Monte Carlo approximation of the Fourier representation

$$
f(x) = \int_{\mathbb{R}^d} \hat{f}(\omega) e^{i \omega \cdot x} dx
$$

using $\bar{c}_{\ell k} = \hat{f}(\omega_k')/(LK \bar{p}'(\omega_k'))$ and the following two lemmas. To obtain a corresponding representation for a deep residual network requires more work, using an optimal control problem for infinite number of nodes and layers presented in Section 4 and an error representation in Section 5 where an analogous Monte Carlo approximation is applied.

**Lemma 3.1.** Assume that $\omega_j, j = 1, \ldots, J$, are independent identically distributed with density $p : \mathbb{R}^d \rightarrow [0, \infty)$, then the mean, variance and kurtosis for the Monte Carlo approximation
\frac{1}{J} \sum_{j=1}^{J} \frac{a(\omega_j)}{p(\omega_j)} \text{ satisfies } E\left[ \sum_{j=1}^{J} \frac{a(\omega_j)}{J p(\omega_j)} \right] = \int_{\mathbb{R}^d} a(\omega) d\omega ,

E[ | \sum_{j=1}^{J} \frac{a(\omega_j)}{J p(\omega_j)} - \int_{\mathbb{R}^d} a(\omega) d\omega |^2 ] = J^{-1} \left( \int_{\mathbb{R}^d} \frac{|a(\omega)|^2}{p(\omega)} d\omega - \left( \int_{\mathbb{R}^d} a(\omega) d\omega \right)^2 \right),

E[ | \sum_{j=1}^{J} \frac{a(\omega_j)}{J p(\omega_j)} - \int_{\mathbb{R}^d} a(\omega) d\omega |^4 ] = J^{-2} \left( \int_{\mathbb{R}^d} \frac{|a(\omega)|^2}{p(\omega)} d\omega - \left( \int_{\mathbb{R}^d} a(\omega) d\omega \right)^2 \right)^2 \nonumber

+ J^{-3} \int_{\mathbb{R}^d} \frac{a(\omega)}{p(\omega)} - \int_{\mathbb{R}^d} a(\omega') d\omega' \right)^4 p(\omega) d\omega .

\text{Proof.} The proof is well known, and is included here for completeness. We have the expected value

\bar{E}_\omega \left[ \sum_{j=1}^{J} \frac{a(\omega_j)}{J p(\omega_j)} \right] = \int_{\mathbb{R}^d} \sum_{j=1}^{J} \frac{a(\omega_j)}{J p(\omega_j)} \prod_{k=1}^{J} p(\omega_k) d\omega_k = \int_{\mathbb{R}^d} a(\omega) d\omega .

The variance of this Monte Carlo approximation satisfies

\bar{E}_\omega \left[ | \sum_{j=1}^{J} \frac{a(\omega_j)}{J p(\omega_j)} - \int_{\mathbb{R}^d} a(\omega) d\omega |^2 \right] \nonumber

= \int_{\mathbb{R}^d} \left( \sum_{j=1}^{J} \frac{a(\omega_j)}{J p(\omega_j)} - \int_{\mathbb{R}^d} a(\omega) d\omega \right)^2 \prod_{k=1}^{J} p(\omega_k) d\omega_k

= J^{-2} \int_{\mathbb{R}^d} \sum_{j=1}^{J} \sum_{i=1}^{J} \frac{a(\omega_j)}{p(\omega_j)} - \int_{\mathbb{R}^d} a(\omega) d\omega \frac{a(\omega_i)}{p(\omega_i)} - \int_{\mathbb{R}^d} a(\omega) d\omega \prod_{k=1}^{J} p(\omega_k) d\omega_k \nonumber

= J^{-2} \int_{\mathbb{R}^d} \sum_{j=1}^{J} \frac{a(\omega_j)}{p(\omega_j)} - \int_{\mathbb{R}^d} a(\omega) d\omega \right)^2 \prod_{k=1}^{J} p(\omega_k) d\omega_k \nonumber

= J^{-1} \left( \int_{\mathbb{R}^d} \frac{|a(\omega)|^2}{p(\omega)} d\omega - \left( \int_{\mathbb{R}^d} a(\omega) d\omega \right)^2 \right) .

The estimate of the fourth moment is obtained similarly. \hfill \Box

The following lemma is a classical result in optimal importance sampling.

Lemma 3.2. The optimal probability density

\begin{align*}
  p_*(\omega) &= \frac{|g(\omega)|}{\int_{\mathbb{R}^d} |g(\omega')| d\omega'} .
\end{align*}

is the solution of the minimization problem

\begin{align*}
  \min_{\int_{\mathbb{R}^d} p(\omega)d\omega = 1} \int_{\mathbb{R}^d} \frac{|g(\omega)|^2}{p(\omega)} d\omega .
\end{align*}
Proof. The change of variables $p(\omega) = q(\omega)/\int_{\mathbb{R}^d} q(\omega) d\omega$ implies $\int_{\mathbb{R}^d} p(\omega) d\omega = 1$, for any $q : \mathbb{R}^d \to [0, \infty)$. We define for any $v : \mathbb{R}^d \to \mathbb{R}$ and $\varepsilon$ close to zero

$$H(\varepsilon) := \int_{\mathbb{R}^d} \frac{|g(\omega)|^2}{q(\omega) + \varepsilon v(\omega)} d\omega \int_{\mathbb{R}^d} q(\omega) + \varepsilon v(\omega) d\omega.$$  

At the optimum we have

$$H'(0) = \int_{\mathbb{R}^d} \frac{|g(\omega)|^2 v(\omega)}{q^2(\omega)} d\omega \int_{\mathbb{R}^d} q(\omega) d\omega' + \int_{\mathbb{R}^d} \frac{|g(\omega')|^2}{q(\omega')} d\omega' \int_{\mathbb{R}^d} v(\omega) d\omega' = c_1 - c_2 \int_{\mathbb{R}^d} \frac{|g(\omega)|^2}{q^2(\omega)} v(\omega) d\omega$$

and the optimality condition $H'(0) = 0$ implies $q(\omega) = \sqrt{\frac{c_1}{c_2}} |g(\omega)|$. Consequently the optimal density becomes

$$p_*(\omega) = \frac{|g(\omega)|}{\int_{\mathbb{R}^d} |g(\omega')|d\omega'}.$$  

□

4. An optimal control solution

In this section we motivate (2.2) and (2.3) using a solution to an optimal control problem related to (1.10) with infinite number of nodes and layers. The complete proof is given in Section 5.

In the limit of infinite $L$ and $K$ with

$$\tilde{b}_{\ell k} \simeq \frac{\hat{b}(t_{\ell k}, \omega_{\ell k})}{L K p(t_{\ell k}, \omega_{\ell k})} \quad \text{and} \quad \tilde{c}_{\ell k} \simeq \frac{\hat{c}(t'_{\ell k}, \omega'_{\ell k})}{L K p'(t'_{\ell k}, \omega'_{\ell k})}$$

the deep residual neural network problem (1.10), with the scaling $\delta = \tilde{\delta}$, becomes the optimal control problem

$$\min_{\hat{b}:[0,1] \times \mathbb{R} \to \mathbb{C}, \hat{c}:[0,1] \times \mathbb{R}^d \to \mathbb{C}} \mathbb{E}_{xy} \left[ |z_1 - (y - \beta(x))|^2 + \tilde{\delta} \int_0^1 |\alpha(t, z_t; x)|^2 dt \right],$$

subject to

$$\frac{dz_t}{dt} = \alpha(t, z_t; x),$$

$$z_0 = 0.$$

We recall the definition of $\alpha(t, z_t; x)$

$$\alpha(t, z_t; x) = \text{Re} \int_{\mathbb{R}} \tilde{b}(t, \omega) e^{i\omega \cdot z_t} d\omega + \text{Re} \int_{\mathbb{R}^d} \tilde{c}(t, \omega) e^{i\omega \cdot x} d\omega.$$  

The motivation for the transformation with $\beta$, where $z_0 = 0$ and $z_1 \simeq y - \beta(x)$, is that our proof requires $\frac{dz_t}{dt}$ to be small compared to one. By choosing $\beta(x)$ to be a neural network approximation of $f(x)$, i.e., $\beta^*(x)$, the difference $y - \beta^*(x)$ becomes sufficiently small.
The noiseless version of (4.1) is the optimal control problem

\[
\min_{\alpha: [0,1] \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}} \mathbb{E}_x \left[ |\tilde{z}_1 - (f(x) - \beta(x))|^2 + \delta \int_0^1 |\alpha(t, \tilde{z}_t; x)|^2 \, dt \right]
\]

subject to

\[
\frac{d\tilde{z}_t}{dt} = \alpha(t, \tilde{z}_t; x), \quad t > 0,
\]
\[
\tilde{z}_0 = 0.
\]

(4.2)

The optimal control problem (4.2) can be solved explicitly as described in Lemma 4.1. This explicit solution is used to derive the bounds (2.2) and (2.3) as follows. The error estimate in Theorem 2.1 is based on an estimate of the difference \( \bar{z}_L - \tilde{z}_1 \), using the optimal solution, \( \tilde{z} \), to (4.2) with the optimal control written as

(4.3)

\[
\alpha(t, \bar{z}_t; x) = \text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega \cdot \bar{z}_t} \, d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega' \cdot x} \, d\omega,
\]

which includes dependence on both \( \bar{z}_t \) and \( x \). This function \( \bar{z} \) is a feasible solution \( z \) to (4.1), since it satisfies the differential equation constraint in (4.1). Its relation to the deep residual neural network problem (1.10) and (1.15) is through Monte Carlo quadrature of the integrals, namely

(4.4)

\[
\text{Re} \sum_{k=1}^K \frac{\hat{b}_{tk} e^{i\omega_{tk} \cdot \bar{z}_t}}{LKP(t_{tk}, \omega_{tk})} + \text{Re} \sum_{k=1}^K \frac{\hat{c}_{tk} e^{i\omega'_{tk} \cdot x}}{LKP'(t'_{tk}, \omega'_{tk})},
\]

where \( \bar{z}_t := \bar{z}(t) \) with \( t = Q^{-1}(\ell) \) and

(4.5)

\[
\hat{b}_{tk} = \hat{b}(t_{tk}, \omega_{tk}) \quad \text{and} \quad \hat{c}_{tk} = \hat{c}(t'_{tk}, \omega'_{tk}).
\]

Below we estimate this Monte Carlo quadrature error. The other part of the error for the estimation in Theorem 2.1, including the difference of \( \bar{z}_L \) and \( \tilde{z}_1 \), based on the values of \( \hat{b}_{tk} \) and \( \hat{c}_{tk} \) obtained from (4.3), is studied in Section 5.

Lemma 4.1. For any nonnegative penalization parameter \( \delta \) the optimal control solution to (4.2) is

\[
\alpha(t, \bar{z}_t; x) = \frac{f(x) - \beta(x)}{\delta + 1}
\]

with the optimal path given by a linear function from initial data to target value as

\[
\bar{z}_t = \frac{t}{1 + \delta} \left( f(x) - \beta(x) \right),
\]
\[
\frac{d\bar{z}_t}{dt} = \frac{f(x) - \beta(x)}{1 + \delta} = \frac{\bar{z}_t}{t},
\]

and the value

\[
\min_{\alpha: [0,1] \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}} \mathbb{E}_x \left[ |\tilde{z}_1 - f(x)|^2 \right] = \mathbb{E}_x \left[ |f(x) - \beta(x)|^2 \right] \frac{\delta^2}{(1 + \delta)^2}.
\]

Proof. We show the result for \( \delta > 0 \) and note that the case \( \delta = 0 \) can be treated by taking the limit \( \delta \to 0 \). Since the control \( \alpha(t, \tilde{z}_t(x); x) \) is allowed to depend on \( x \), the minimum in
\( (4.2) \) can be performed with respect to each data point \( x \) individually, so that \( (4.2) \) implies
\[
\min_{\alpha: [0,1] \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}} \left\{ |\tilde{z}_1 - (f(x) - \beta(x))|^2 + \delta \int_0^1 |\alpha(s, \tilde{z}_s; x)|^2 ds \right\}
\]
subject to \( \frac{d\tilde{z}_t}{dt} = \alpha(t, \tilde{z}_t; x) \), \( t > 0 \),
\( \tilde{z}_0 = 0 \).

Its Lagrangian becomes
\[
\mathcal{L}(\tilde{z}, \lambda, \alpha) := |\tilde{z}_1 - (f(x) - \beta(x))|^2 + \delta \int_0^1 |\alpha t|^2 dt + \int_0^1 \lambda_t \cdot (\alpha_t - \frac{d\tilde{z}_t}{dt}) dt
\]
with the corresponding Lagrange multiplier condition
\[
\frac{d\lambda_t}{dt} = 0, \quad t < 1,
\]
\( \lambda_1 = 2 \left( \tilde{z}_1 - (f(x) - \beta(x)) \right) \),
and the Pontryagin principle
\[
\alpha_t = \arg \min_{a \in \mathbb{R}^d} (\lambda_t \cdot a + \delta |a|^2).
\]
The solution becomes
\[
\alpha_t = -\frac{1}{\delta} \left( \tilde{z}_1 - (f(x) - \beta(x)) \right),
\]
and we obtain
\[
\tilde{z}_t = -\frac{t}{\delta} \left( \tilde{z}_1 - (f(x) - \beta(x)) \right),
\]
and
\[
\tilde{z}_1 = \frac{f(x) - \beta(x)}{1 + \delta}.
\]
Therefore we have
\[
\alpha_t = \frac{f(x) - \beta(x)}{1 + \delta},
\]
and
\[
\frac{d\tilde{z}_t}{dt} = \frac{(f(x) - \beta(x))}{1 + \delta} = \frac{\tilde{z}_t}{t},
\]
so that a feasible solution for \( (4.1) \) is
\[
(4.8) \quad \Re \int_{\mathbb{R}} \hat{b}(t, \omega)e^{i\omega \tilde{z}_t} d\omega + \Re \int_{\mathbb{R}^d} \hat{c}(t, \omega)e^{i\omega \cdot x} d\omega = \frac{f(x) - \beta(x)}{\delta + 1} = \frac{\tilde{z}_t}{t}.
\]

Due to the singularity in \( \tilde{z}_t/t \), at \( t = 0 \) in \( (4.8) \), it is for small \( t \) advantageous that the function \( \Re \int_{\mathbb{R}^d} \hat{c}(t, \omega)e^{i\omega \cdot x} d\omega \approx \frac{f(x) - \beta(x)}{\delta + 1} \) and let \( \hat{b}(t, \cdot) = 0 \), while for larger \( t \) it can be better to let
\[
\Re \int_{\mathbb{R}} \hat{b}(t, \omega)e^{i\omega \tilde{z}_t} d\omega = \frac{\tilde{z}_t}{t}.
\]
To minimize the Monte Carlo approximation variance, \( \mathcal{E} \), of (4.3) approximating the integrals in (4.8) with the sum in (4.4) we can choose between these two options, namely we use for \( \gamma : [0, 1] \to [0, 1] \) the convex combination

\[
\text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega)e^{i\omega\hat{\omega}}d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega)e^{i\omega \cdot x}d\omega = \gamma(t)\frac{f(x) - \beta(x)}{\delta + 1} + (1 - \gamma(t))\frac{\overline{z_t}}{t},
\]

and

\[
\text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega)e^{i\omega\hat{\omega}}d\omega = \left(1 - \gamma(t)\right)\frac{\overline{z_t}}{t},
\]

(4.9)

\[
\text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega)e^{i\omega \cdot x}d\omega = \gamma(t)\frac{f(x) - \beta(x)}{\delta + 1},
\]

which by Lemma 3.1 implies

Lemma 4.2. Assume \( \beta(x) = \text{Re} \sum_{k=1}^{K} \frac{f(\omega'_k)e^{i\omega'_k \cdot x}}{Kp(\omega'_k)} \) and let \( \hat{b}_{\ell k} \) and \( \hat{c}_{\ell k} \) be defined by (4.5) and (4.9), for \( k = 1, \ldots, K \) and \( \ell = 1, \ldots, L - 1 \), then

\[
\min_{\gamma : [0, 1] \to [0, 1]} \mathbb{E}_{\omega} \left[ \left| \text{Re} \sum_{\ell=1}^{L-1} \sum_{k=1}^{K} \hat{b}_{\ell k}e^{i\omega\hat{\omega}} + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega)e^{i\omega \cdot x} d\omega \right|^2 \right]
\]

\[
\leq \frac{B'^2_*}{LK}(1 + \log \frac{A_*}{B'_*})^2
\]

for the optimal time dependent densities,

\[
p'(t, \omega) := \bar{p}'(\omega)q'(t) = \begin{cases} \frac{|f(\omega)|}{\|f\|_{L^1([0, t])}} & t < t_* := \min(1, \frac{B'_*}{A_*}) , \\ 0 & t \geq t_* , \end{cases}
\]

\[
p(t, \omega) := \bar{p}(\omega)q(t) = \begin{cases} t^{-1}|\partial_\omega \hat{h}(F\omega)| & t < t_* , \\ \|t^{-1}\partial_\omega \hat{h}(F\omega)\|_{L^1([0, 1])} & t \geq t_* , \end{cases}
\]

\[
A_* := \|\hat{f}\|_{L^1(\mathbb{R}^d)} , \\
B'_* := F\|\partial_\omega \hat{h}(F\omega)\|_{L^1(\mathbb{R})} .
\]

If \( q \) and \( q' \) are constant on their support, the bound \( \frac{B'^2_*}{LK}(1 + \log \frac{A_*}{B'_*})^2 \) in (4.10) is replaced by \( \min(2(AB)^{1/2} - B, A) \) using \( \gamma(t) = 1_{[0, \min(1, \sqrt{B'/A})]}(t) \).

Proof. We note that since \( \beta(x) \) is a given neural network function, replacing \( c(t, x) \) by \( c(t, x) + \beta(x)\frac{\gamma(t)}{1 + \delta} \) does not contribute to the approximation error. To determine \( \hat{b} \) from \( \frac{\overline{z_t}}{t} \) we use that the constant \( F \) is by definition the bound

\[
F = \|f\|_{L^\infty(\mathbb{R}^d)} \leq \int_{\mathbb{R}^d} |\hat{f}(\omega)|d\omega
\]

and since by assumption \( h(z) = 1 \) for \( |z| \leq 1 \), the map \( z \mapsto z h(z/F) \) is the identity map, for \( |z| \leq F \), and its Fourier transform \( \omega \mapsto -i F^2 \partial_\omega \hat{h}(F\omega) \) is a Schwartz function. The variance
of the Monte Carlo error

\[ \mathcal{E}(\gamma) := \mathbb{E}_w \left[ \text{Re} \sum_{\ell=1}^{L-1} \sum_{k=1}^{K} \frac{\hat{b}_{\ell k} e^{i\omega_{\ell k} \cdot x}}{L K p(t_{\ell k}, \omega_{\ell k})} + \text{Re} \sum_{k=1}^{K'} \frac{\hat{c}_{\ell k} e^{i\omega_{\ell k} \cdot x}}{L K p'(t_{\ell k}, \omega'_{\ell k})} \right] \]

\[ - \sum_{\ell=0}^{L-1} \int_{t_{\ell}}^{t_{\ell+1}} \left( \text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega \cdot z_t} d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega \cdot x} d\omega \right) dt \]

which implies the bang-bang control (2.3), i.e. related to (4.4) to define \( \bar{\gamma} \) and (4.8) and defined by the solution \( \tilde{\gamma} \).

To derive an error estimate we choose the discrete amplitudes to be the same as the amplitudes for the time layer values \( \gamma(t) \) in Lemma 4.1, using also the optimal partition (4.9) with \( \gamma(t) = 1_{t < \min(1, B/A_\ast)}(t) \), for optimal time dependent densities, and \( \gamma(t) = 1_{t < \min(1, (B/A)^{1/2})}(t) \) for densities \( q \) and \( q' \) that are constant on their support. Therefore we will use the amplitudes related to (4.4) to define \( \tilde{\gamma} \) from \( \hat{b}_{\ell k} = \hat{b}(t_{\ell k}, \omega_{\ell k}) \) and \( \hat{c}_{\ell k} = \hat{c}(t_{\ell k}, \omega_{\ell k}) \), which are given in (4.5) and (4.8) and defined by the solution \( \tilde{\gamma} = \gamma \).

Theorem 2.1. We denote a feasible solution to (4.1) by \( \gamma(t) \) or \( z_t \). We define, for \( \ell = 0, \ldots, L \), the time layer values

\[ z_{\ell} := z(t_{\ell}), \quad \text{where} \quad t_{\ell} := Q^{-1}(\ell/L). \]

To derive an error estimate we choose the discrete amplitudes to be the same as the amplitudes for the feasible \( z = \tilde{z} \) derived in Lemma 4.1, using also the optimal partition (4.9) with \( \gamma(t) = 1_{t < \min(1, B/A_\ast)}(t) \), for optimal time dependent densities, and \( \gamma(t) = 1_{t < \min(1, (B/A)^{1/2})}(t) \) for densities \( q \) and \( q' \) that are constant on their support. Therefore we will use the amplitudes related to (4.4) to define \( \tilde{\gamma} \) from \( \hat{b}_{\ell k} = \hat{b}(t_{\ell k}, \omega_{\ell k}) \) and \( \hat{c}_{\ell k} = \hat{c}(t_{\ell k}, \omega_{\ell k}) \), which are given in (4.5) and (4.8) and defined by the solution \( \tilde{\gamma} = \gamma \). The aim is to estimate \( \mathbb{E}_{xy}[|\tilde{z}_L^* - (y - \beta^*(x))|^2] \).
where $\bar{z}^*$ is an optimal solution to (1.10). The minimum property of $\bar{z}_L^*$ implies that for any positive $\zeta$ we have
\[ E_{t\omega}[E_{xy}[|\bar{z}_L^* - (y - \beta^*(x))|^2]] \]
\[ \leq E_{t\omega}[E_{xy}[|\bar{z}_L^* - (y - \beta^*(x))|^2 + \delta L \sum_{\ell=1}^{L-1} |\bar{z}_{\ell+1} - \bar{z}_\ell^*|^2]] \]
\[ \leq E_{t\omega}[E_{xy}[|\bar{z}_L^* - (y - \beta^*(x))|^2 + \delta L \sum_{\ell=1}^{L-1} |\bar{z}_{\ell+1} - \bar{z}_\ell|^2]] \]
\[ = E_{t\omega}[E_{xy}[(\bar{z}_L - z_1) + (z_1 - \bar{z}_1) + \bar{z}_1 - (y - \beta^*(x))^2] + O(\delta) \]
\[ \leq (1 + \zeta^2)E_{t\omega}[E_{xy}[|\bar{z}_L - z_1|^2]] \]
\[ + (1 + \zeta^{-2})E_{t\omega}[E_{xy}[(z_1 - \bar{z}_1) + \bar{z}_1 - (y - \beta^*(x))^2]] + O(\delta) . \]

By choosing $z = \bar{z}$, Lemma 4.1 yields
\[ E_{xy}[(z_1 - \bar{z}_1) + \bar{z}_1 - (y - \beta^*(x))^2] \leq 2E_{xy}[|\bar{z}_1 - (f(x) - \beta^*(x))|^2] + 2\epsilon^2 = O(\delta^2 + \epsilon^2) , \]
and we conclude
\[ (5.1) \ E_{t\omega}[E_{xy}[|\bar{z}_L^* - (y - \beta^*(x))^2]] \leq (1 + \zeta^2)E_{t\omega}[E_{xy}[|\bar{z}_L - z_1|^2]] + O(\delta + (\delta^2 + \epsilon^2)(1 + \zeta^{-2})) . \]

It remains to estimate the term $E_{t\omega}[E_{xy}[|\bar{z}_L - z_1|^2]]$, which has four steps:

1. formulate an error representation of the exact path $z_t$ evaluated along the discrete value function for the ordinary difference equation in (1.10),
2. estimate the derivatives of the value functions for the differential equation in (4.1) and the difference equation in (1.10),
3. derive an error estimate for $E_{t\omega}[|z_t - \bar{z}_t|^2]$, using a discrete Gronwall inequality applied to the difference of the dynamics of $\bar{z}_t$ and $z_t$, and
4. use Steps 1, 2, and 3 to derive Monte Carlo quadrature error for
\[ \text{Re} \sum_{\ell=0}^{L-1} \sum_{k=1}^{K} \frac{\hat{b}_{\ell k} e^{i \omega_{\ell k} \cdot \bar{z}_\ell}}{LKp(t_{\ell k}, \omega_{\ell k})} + \text{Re} \sum_{\ell=0}^{L-1} \sum_{k=1}^{K} \frac{\hat{c}_{\ell k} e^{i \omega_{\ell k} \cdot x}}{LKp'(t'_{\ell k}, \omega'_{\ell k})} . \]

Step 1. Error representation] We define
\[ \hat{B}(\bar{z}_t, \ell) := \text{Re} \sum_{k=1}^{K} \frac{\hat{b}_{\ell k} e^{i \omega_{\ell k} \cdot \bar{z}_\ell}}{LKp(t_{\ell k}, \omega_{\ell k})} \]
\[ \hat{C}(\ell) := \text{Re} \sum_{k=1}^{K'} \frac{\hat{c}_{\ell k} e^{i \omega'_{\ell k} \cdot x}}{LKp'(t'_{\ell k}, \omega'_{\ell k})} \]
\[ \hat{D}(\bar{z}_t, \ell) := \hat{B}(\bar{z}_t, \ell) + \hat{C}(\ell) . \]

Fix a data point $(x, y)$, then define for this $x$ and for any $z \in \mathbb{R}$ the discrete value function
\[ \bar{u}(z, \bar{\ell}) = \bar{z}_L , \]
\[ \bar{z}_{\ell+1} = \bar{z}_\ell + \hat{B}(\bar{z}_\ell, \ell) + \hat{C}(\ell) , \]
\[ \bar{z}_\ell = z . \]
We have
\[ z_L - \bar{z}_L = \bar{u}(z_L, L) - \bar{u}(z_0, 0) \]
\[ = \sum_{\ell=0}^{L-1} (\bar{u}(z_{\ell+1}, \ell + 1) - \bar{u}(z_\ell, \ell)) \]
and by construction there holds for any \( z \)
\[ \bar{u}(z, \ell) = \bar{u}(z + \bar{D}(z, \ell), \ell + 1) . \]

Introducing for \( \ell = 0, \ldots, L \) the notation
\[ B(\bar{z}_\ell, \ell) := \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega \cdot \bar{z}_t} d\omega dt , \]
\[ C(\ell) := \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega \cdot x} d\omega dt , \]
\[ D(\bar{z}_\ell, \ell) := B(\bar{z}_\ell, \ell) + C(\ell) , \]
telescoping summation implies
\[ z_L - \bar{z}_L = \sum_{\ell=0}^{L-1} (\bar{u}(z_\ell + D(z_\ell, \ell), \ell + 1) - \bar{u}(z_\ell + \bar{D}(z_\ell, \ell), \ell + 1)) \]
\[ = \sum_{\ell=0}^{L-1} \int_0^1 \partial_z \bar{u}(z_\ell + s(D(z_\ell, \ell) - \bar{D}(z_\ell, \ell)), \ell + 1) ds \cdot (D(z_\ell, \ell) - \bar{D}(z_\ell, \ell)) \]
\[ = \sum_{\ell=0}^{L-1} \partial_z \bar{u}(z_\ell) \cdot (D(z_\ell, \ell) - \bar{D}(z_\ell, \ell)) , \]
where, for the sake of brevity, we defined
\[ \partial_z \bar{u}(z_\ell) = \int_0^1 \partial_z \bar{u}(z_\ell + s(D(z_\ell, \ell) - \bar{D}(z_\ell, \ell)), \ell + 1) ds . \]

Next we let
\[ u(z, \ell) = z_L = z_{t \mid t = 1} , \]
where
\[ \frac{dz_t}{dt} = \text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega \cdot \bar{z}_t} d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega \cdot x} d\omega , \quad t > t_\ell , \]
\[ z_{t_\ell} = z . \]
We obtain an error representation based on the exact optimal path \( z_\ell \) evaluated along the discrete value function \( \bar{u} \)

\[
\mathbb{E}_{t,\omega}[|z_L - \bar{z}_L|^2] = \mathbb{E}_{t,\omega} \left[ \left( \sum_{\ell=0}^{L-1} \partial_z \bar{u}(z_\ell) \cdot (D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)) \right)^2 \right]
\]

\[
= \mathbb{E} \left[ \left( \sum_{\ell=0}^{L-1} \partial_z u(z_\ell, \ell + 1) \cdot (D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)) + \sum_{\ell=0}^{L-1} (\partial_z \bar{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1)) \cdot (D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)) \right)^2 \right]
\]

(5.2)

\[
\leq (1 + \zeta^2) \mathbb{E}_{t,\omega} \left[ \left( \sum_{\ell=0}^{L-1} \partial_z u(z_\ell, \ell + 1) \cdot (D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)) \right)^2 \right]
\]

\[
+ (1 + \zeta^{-2}) \mathbb{E}_{t,\omega} \left[ \left( \sum_{\ell=0}^{L-1} (\partial_z \bar{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1)) \cdot (D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)) \right)^2 \right]
\]

for any \( \zeta > 0 \). Introducing

\[
\tilde{D}(z_\ell, \ell) := \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} d\omega dt + \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega x} d\omega dt
\]

we have

\[
D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell) = D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell) + \tilde{D}(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)
\]

\[
= \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} d\omega dt - \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} d\omega dt
\]

\[
+ \tilde{D}(z_\ell, \ell) - \tilde{D}(z_\ell, \ell),
\]

(5.3)

\[
\tilde{D}(z_\ell, \ell) - \tilde{D}(z_\ell, \ell) = \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} d\omega dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{b}_{ik}}{L K p(t_{\ell k}, \omega_{\ell k})} e^{i\omega_{\ell k} z_\ell}
\]

\[
+ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega x} d\omega dt - \text{Re} \sum_{k=1}^{K'} \frac{\hat{c}_{\ell k}}{L K' p'(t'_{\ell k}, \omega'_{\ell k})} e^{i\omega'_{\ell k} x}.
\]

The deterministic \( \xi_\alpha \) has the representation

(5.4)

\[
L^{-1} \xi_\alpha = \int_{t_\ell}^{t_{\ell+1}} b(t, z_\ell) dt - \int_{t_\ell}^{t_{\ell+1}} b(t, z_\ell) dt
\]

with the bound \( |\xi_\alpha| = \mathcal{O}(L^{-1}) \). In Step 3, we use \( \mathbb{E}_{t,\omega}[\tilde{D}(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)] = 0 \) and Lemma 3.1 to establish \( \mathbb{E}_{t,\omega}[L^2|\tilde{D}(z_\ell, \ell) - \tilde{D}(z_\ell, \ell)|^2] = \mathcal{O}(K^{-1}) \). We shall show in Step 4 that the first term in the right hand side of (5.2) is \( \mathcal{O}(L^{-1} K^{-1}) \) by Monte-Carlo quadrature in space-time, using \( \mathbb{E}_{t,\omega}[\sum_{\ell=0}^{L-1} \partial_z u(z_\ell, \ell + 1) \cdot (D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell))] = 0 \). Step 3 estimates the second term in the right hand side of (5.2). The next step estimates the derivatives of \( u \) and \( \bar{u} \).
Step 2. [Derivatives of the value functions] The definition \( u(z, \ell) = z_1 \) and
\[
\frac{dz_s}{ds} = \text{Re} \int_{\mathbb{R}} \hat{b}(s, \omega) e^{i\omega \cdot z_s} d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(s, \omega) e^{i\omega' \cdot x} d\omega, \quad s > t
\]
\( z_t = z \),

imply that \( \partial z u(z, \ell) = z_1' \), where the first variation \( z_1' := \frac{\partial z_s}{\partial z_1} \) solves
\[
\frac{dz_{s,t}'}{ds} = \text{Re} \int_{\mathbb{R}} i \hat{b}(s, \omega) e^{i\omega \cdot z_s} \omega z_{s,t}' d\omega = \partial_z b(s, z) z_{s,t}' , \quad s > t, \ell
\]
\( z_{t',t} = 1 \).

This differential equation has the solution
\[
(5.5) \quad \partial z u(z, \ell) = e^{\int_{t'}^t \partial_z b(s, z_s) ds}.
\]

To similarly obtain a representation for the gradient of the discrete value function we use that \( \partial \bar{z} u(z, \ell) = z_{L,\ell}' \), where the discrete variation \( z_{L,\ell}' := \frac{\partial \bar{z}_s}{\partial \bar{z}_1} \) satisfies
\[
\frac{dz_{s,\ell}'}{ds} = \text{Re} \sum_{k=1}^{K} \frac{i \hat{b}_{lk}}{LK \hat{p}(t_{lk}, \omega_{lk})} e^{i\omega_{lk} \cdot \bar{z}_s} \omega_{lk} z_{s,\ell}' 
\]
\( z_{t,\ell}' = 1 \),

where we write
\[
(1 + L^{-1} \hat{b}_\ell(\bar{z}_\ell)) z_{L,\ell}' := z_{L,\ell}' + \text{Re} \sum_{k=1}^{K} \frac{i \hat{b}_{lk}}{LK \hat{p}(t_{lk}, \omega_{lk})} e^{i\omega_{lk} \cdot \bar{z}_s} \omega_{lk} z_{s,\ell}' .
\]

Thus we have the solution
\[
(5.6) \quad z_{L,\ell}' = \prod_{t=\ell}^{L-1} (1 + L^{-1} \hat{b}_t(\bar{z}_t)) .
\]

We also obtain the second derivative estimate
\[
(5.7) \quad |\partial^2 z u(z, x, \ell)| \leq \int_{t'}^1 |\partial^2 z b(s, z)\big| e^{\int_{t'}^s |\partial_z b(s, z)| ds} e^{\int_{t'}^s |\partial_z b(s, z)| ds} ds
\]
\[
Step 3. [Gronwall inequality] The second term in the right hand side of (5.2) requires an estimate of \( z_t - z_\ell \). Let \( \varepsilon_\ell := z_t - z_\ell \) with \( \varepsilon_1 = z_1 - z_\ell = 0 \). We will first use a discrete Gronwall inequality, see Lemma 5.1, to estimate \( \varepsilon_\ell \) and then estimate \( \partial \bar{z} \bar{u} - \partial z u \).
Estimate of $\varepsilon_\ell = z_\ell - z_\ell$. We have by the dynamics (1.10) and (4.1)

$$
\varepsilon_{\ell+1} = \varepsilon_\ell + \text{Re} \sum_{k=1}^K \frac{\hat{b}_{tk}}{LKp(t_{tk}, \omega_{tk})} (e^{i\omega_{tk}z_\ell} - e^{i\omega_{tk}z_\ell})
+ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} d\omega dt - \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} d\omega dt
=: L^{-1}\xi_a
$$

$$
+ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} d\omega dt - \text{Re} \sum_{k=1}^K \frac{\hat{b}_{tk}}{LKp(t_{tk}, \omega_{tk})} e^{i\omega_{tk}z_\ell}
=: L^{-1}\xi_b(\ell)
$$

$$
+ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega x} d\omega dt - \text{Re} \sum_{k=1}^K \frac{\hat{c}_{tk}}{LKp'(t_{tk}', \omega_{tk}')} e^{i\omega_{tk}'x}
=: L^{-1}\xi_c(\ell)
$$

$$=: \varepsilon_\ell + \text{Re} \sum_{k=1}^K \frac{\hat{b}_{tk}}{LKp(t_{tk}, \omega_{tk})} e^{i\omega_{tk}z_\ell} (1 - e^{-i\omega_{tk}z_\ell}) + L^{-1}(\xi_a + \xi_b + \xi_c).
$$

The term $L^{-1}\xi_a$ is a deterministic quadrature problem (5.4) and since $d b(t, z_\ell)/dt$ is bounded we have $|\xi_a| = O(L^{-1})$. Using the Monte Carlo quadrature estimate in Lemma 3.1 to obtain for $j = b, c$

$$
\xi_a = O(L^{-1}),
\mathbb{E}_{t_\omega}[\xi] = 0,
\mathbb{E}_{t_\omega}[|\xi|^2] = O(K^{-1}),
\mathbb{E}_{t_\omega}[|\xi|^4] = O(K^{-2}).
$$

The next step is to estimate the sum over $k$ in the right hand side of (5.8). We have

$$|1 - e^{-i\omega_{tk}z_\ell}| \leq |\omega_{tk}||\varepsilon_\ell|$$

which implies

$$a_\ell := \sum_{k=1}^K \frac{\hat{b}_{tk}}{LKp(t_{tk}, \omega_{tk})} e^{i\omega_{tk}z_\ell} (1 - e^{-i\omega_{tk}z_\ell}) \leq \sum_{k=1}^K \frac{\hat{b}_{tk}}{LKp(t_{tk}, \omega_{tk})} |\omega_{tk}|.$$

Next we determine a probability that $a_\ell$ are bounded by a number $a$ for $\ell = 0, \ldots, L$. By the Chernoff bound in Lemma 5.2 based on $|\hat{b}(t_{tk}, \omega_{tk})| |\omega_{tk}|$ being bounded, we have

$$|a_\ell| \leq \sum_{k=1}^K \frac{\hat{b}_{tk}}{Kp(t_{tk}, \omega_{tk})} |\omega_{tk}| = \int_{\mathbb{R}} |\hat{b}(t_{tk}, \omega)| |\omega| d\omega + K^{-1} \nu_\ell$$

where $\nu_\ell$ is a random variable where $\mathbb{P}(\frac{|\nu_\ell|}{K} > \alpha)$ is bounded by $e^{-\alpha K}$. By independence becomes

$$\mathbb{P}(\max_\ell \frac{|\nu_\ell|}{K} > \alpha) \leq L e^{-\alpha K}.$$
for some (other) positive constant $c$.

We obtain for any $\zeta$, in particular for $\zeta = L^{-1/2}$,
\begin{equation}
|\varepsilon_{\ell+1}|^2 = |\varepsilon_{\ell}| + \Re \sum_{k=1}^{K} \frac{\hat{b}_{lk}}{L K p(t_{\ell k}, \omega_{\ell k})} e^{i \omega_{\ell k} |\varepsilon_{\ell}|} (1 - e^{-i \omega_{\ell k} |\varepsilon_{\ell}|}) + L^{-1} (\xi_a + \xi_b + \xi_c)^2
\end{equation}
(5.10)
\begin{align*}
&\leq |\varepsilon_{\ell}|^2 (1 + L^{-1} a_\ell)^2 (1 + \zeta^2) + (1 + \zeta^{-2}) L^{-2} |\xi_a + \xi_b + \xi_c|^2 \\
&\leq |\varepsilon_{\ell}|^2 (1 + L^{-1} a_\ell)^2 (1 + L^{-1}) + (1 + L) L^{-2} |\xi_a + \xi_b + \xi_c|^2.
\end{align*}

When all $a_\ell$ are bounded by $\alpha$, we can apply Gronwall’s inequality in Lemma 5.1 to obtain $|\varepsilon_{\ell}|^2 = O(\sum_{\ell=0}^{L-1} |\xi_a(\ell) + \xi_b(\ell) + \xi_c(\ell)|^2 L^{-1})$. In the complement set, which has a small probability bounded by $Le^{-cK\alpha^2}$, the differences $|\varepsilon_{\ell}|$ are uniformly bounded, since by assumptions the data $|f(x)|$ are bounded in the maximum norm, and $\|\frac{\partial}{\partial \ell} b(F(\ell))\|_{L^\infty(\mathbb{R})} + \|\frac{\partial}{\partial \ell} \|_{L^\infty(\mathbb{R}^d)}$ are bounded, which implies that $\|\varepsilon(x)\|_{L^\infty(\mathbb{R})}$ is bounded. Consequently there is a positive constant $c$ such that $\mathbb{E}_{t,\omega} |\varepsilon_{\ell}|^2 = O(L^{-2} + K^{-1} + Le^{-cK})$, for all $\ell$. Squaring (5.10) yields the recursion
\begin{equation}
|\varepsilon_{\ell+1}|^4 \leq |\varepsilon_{\ell}|^4 (1 + L^{-1} a_\ell)^4 (1 + L^{-1})^3 (1 + L)^3 L^{-4} |\xi_a + \xi_b + \xi_c|^4
\end{equation}
(5.11)
and a similar Gronwall estimate implies then that there is a positive constant $c$ such that
\begin{align*}
\mathbb{E}_{t,\omega}[|\varepsilon_{\ell}|^2] &= O(L^{-2} + K^{-1} + Le^{-cK}) , \\
\mathbb{E}_{t,\omega}[|\varepsilon_{\ell}|^4] &= O(L^{-4} + K^{-2} + Le^{-cK}) .
\end{align*}
(5.12)

Estimate of $\partial_z \bar{u} - \partial_z u$. To estimate $\partial_z \bar{u} - \partial_z u$ we make the splitting
\begin{align}
\partial_z \bar{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1) &= \int_0^1 \partial_z \bar{u} \left( z_\ell + s \left( D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \right), \ell + 1 \right) ds - \partial_z u(z_\ell, \ell + 1) \\
&= \int_0^1 \left[ \partial_z \bar{u} \left( z_\ell + s \left( D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \right), \ell + 1 \right) \\
&\quad - \partial_z u \left( z_\ell + s \left( D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \right), \ell + 1 \right) \right] ds \\
&\quad + \int_0^1 [\partial_z u \left( z_\ell + s \left( D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \right), \ell + 1 \right) - \partial_z u(z_\ell, \ell + 1)] ds .
\end{align}
(5.13)

The second term has the estimate
\begin{equation}
|\int_0^1 [\partial_z u \left( z_\ell + s \left( D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \right), \ell + 1 \right) - \partial_z u(z_\ell, \ell + 1)] ds| \\
\leq \|\partial_z^2 u\|_{L^\infty} |D(z_\ell, \ell) - \bar{D}(z_\ell, \ell)|
\end{equation}
(5.14)
where we use (5.7) to bound the second derivatives of $u$. To bound the first term in the right hand side we use for each $s \in [0, 1]$ the path $z(t; s)$ that solves the differential equation (4.1), with the given $\hat{b}(t, \omega)$ and $\hat{c}(t, \omega)$ obtained from $\bar{z}$, and at time $t_{\ell+1}$ the path starts with value $z_\ell + s \left( D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \right)$. Then we estimate the difference $\partial_z \bar{u} - \partial_z u$ along the same such paths $z(t; s)$. At all time levels $t_\ell$, $\ell' = \ell, \ldots, L$ we still denote the path value $z_\ell'$. We have by (5.5)
\begin{equation}
\partial_z u(z_\ell, \ell + 1) = e^{\int_{t_{\ell+1}}^{t_{\ell+1}} b(s, z_s) ds}
\end{equation}
and with probability $1 - L e^{-cK\alpha^2}$ by (5.6) and (5.8)

$$
\frac{\partial_z \tilde{u}(z_\ell)}{\partial_z u(z_\ell, \ell + 1)} = \mathcal{O}(L^{-2}) + \mathcal{O}\left(\sum_{\ell' = \ell}^{L-1} |\epsilon_{\ell'}| + |\xi_b(\ell')| \right)
$$

As in (5.8) we obtain

$$
\text{Re} \left( \sum_{\ell' = \ell}^{L-1} \sum_{k=1}^{K} \frac{\hat{b}_{\ell' k} e^{|i\omega_{\ell' k} z_{\ell'}}}{L K p(t_{\ell' k}, \omega_{\ell' k})} \right)
$$

so that with probability $1 - e^{-cK\alpha^2}$

$$
|\partial_z \tilde{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1)|^2 = \mathcal{O}(L^{-2}) + \mathcal{O}\left(\sum_{\ell' = \ell}^{L-1} |\epsilon_{\ell'}| + |\xi_b(\ell')| \right)
$$

and by (5.12), (5.13) and (5.14)

(5.15)

$$
\begin{align*}
\mathbb{E}_{t, \omega}[||\partial_z \tilde{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1)||^2] &= \mathcal{O}(K^{-1} + L^{-2} + Le^{-cK}), \\
\mathbb{E}_{t, \omega}[||\partial_z \tilde{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1)||^4] &= \mathcal{O}(K^{-2} + L^{-4} + Le^{-cK}), \\
\mathbb{E}_{t, \omega}[||D(z_\ell, \ell) - D(z_\ell, \ell)||^2] &= L^{-2}\mathcal{O}(K^{-1} + L^{-2}), \\
\mathbb{E}_{t, \omega}[||D(z_\ell, \ell) - D(z_\ell, \ell)||^4] &= L^{-4}\mathcal{O}(K^{-2} + L^{-4}).
\end{align*}
$$

The second term in the right hand side of (5.2) has the estimate

$$(1 + \zeta^{-2})\mathbb{E}_{t, \omega}\left[\left(\sum_{\ell = 0}^{L-1} (\partial_z \tilde{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1)) \cdot (D(z_\ell, \ell) - \tilde{D}(z_\ell, \ell))\right)^2\right].$$
Introducing the notation \( \Delta u_\ell := \partial_z \bar{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1) \) and \( \Delta D_\ell := D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \) we have

\[
\mathbb{E}_{t_\omega} \left[ \left( \sum_{\ell=0}^{L-1} \left( \partial_z \bar{u}(z_\ell) - \partial_z u(z_\ell, \ell + 1) \right) \cdot \left( D(z_\ell, \ell) - \bar{D}(z_\ell, \ell) \right) \right)^2 \right]
\]

\[
= \sum_{\ell=0}^{L-1} \sum_{\ell'=0}^{L-1} \mathbb{E}_{t_\omega} \left[ (\Delta u_\ell \cdot \Delta D_\ell)(\Delta u_{\ell'} \cdot \Delta D_{\ell'}) \right]
\]

\[
\leq \sum_{\ell=0}^{L-1} \sum_{\ell'=0}^{L-1} \left( \mathbb{E}_{t_\omega}[|\Delta u_\ell|^2] \mathbb{E}_{t_\omega}[|\Delta u_{\ell'}|^2] \mathbb{E}_{t_\omega}[|\Delta D_\ell|^2] \mathbb{E}_{t_\omega}[|\Delta D_{\ell'}|^2] \right)^{1/2}
\]

\[
= L^2 \mathcal{O}(K^{-1} + L^{-2} + L e^{-cK}) \mathcal{O}(K^{-1} + L^{-2}) L^{-2} = \mathcal{O}(K^{-2} + L^{-4} + L e^{-cK}),
\]

using (5.15). The next step estimates the first term in the right hand side of (5.2).

**Step 4.** [Monte Carlo quadrature error] We will see that provided \( L \ll K \ll L^3 \), the generalization error is dominated by

\[
R_0 := \mathbb{E}_{t_\omega} \left[ \left( \sum_{\ell=0}^{L-1} \partial_z u(z_\ell, \ell + 1) \cdot \left( D(z_\ell) - \bar{D}(z_\ell) \right) \right)^2 \right]
\]

\[
= \mathbb{E}_{t_\omega} \left[ \left( \sum_{\ell=0}^{L-1} \partial_z u(z_\ell, \ell + 1) \times \right.ight.
\]

\[
\times \left\{ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_\ell} \, d\omega \, dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{b}_{tk}}{LKp(t_{tk}, \omega_{tk})} e^{i\omega_{tk} z_\ell} \right. \]

\[
\left. + \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}^d} \hat{c}(t, \omega) e^{i\omega x} \, d\omega \, dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{c}_{tk}}{LKp'(t'_{tk}, \omega'_{tk})} e^{i\omega'_{tk} x} \right) \}
\]

\[
\left. \right)^2 \right].
\]
The sum over $\ell$ in $R_0$ can for any $\zeta \in \mathbb{R}$ be split (to separate out the mean zero terms) as in (5.3)

$$R_0 = \mathbb{E}_{t_\omega}\left[\left(\sum_{\ell=0}^{L-1} \partial_2 u(z_\ell, \ell + 1) \{D(z_\ell) - \tilde{D}(z_\ell)\} + \sum_{\ell=0}^{L-1} \partial_2 u(z_\ell, \ell + 1) \cdot (\tilde{D}(z_\ell) - \bar{D}(z_\ell))\right)^2\right]$$

\leq (1 + \zeta^2) \mathbb{E}_{t_\omega} \left[\left(\sum_{\ell=0}^{L-1} \partial_2 u(z_\ell, \ell + 1) \cdot (\tilde{D}(z_\ell) - \bar{D}(z_\ell))\right)^2\right]

\leq (1 + \zeta^2) \mathbb{E}_{t_\omega} \left[\left(\sum_{\ell=0}^{L-1} \partial_2 u(z_\ell, \ell + 1) \cdot (D(z_\ell) - \bar{D}(z_\ell))\right)^2\right]

\leq (1 + \zeta^2) \mathbb{E}_{t_\omega} \left[\left(\sum_{\ell=0}^{L-1} \partial_2 u(z_\ell, \ell + 1) \times\right.ight.

\times \left\{ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i \omega \cdot z_\ell} d\omega dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{b}_{tk}}{L K p(t_{ck}, \omega_{tk})} e^{i \omega_{tk} \cdot z_\ell}

+ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}^4} \hat{c}(t, \omega) e^{i \omega \cdot x} d\omega dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{c}_{tk}}{L K p'(t_{ck}, \omega_{tk})} e^{i \omega_{tk}' \cdot x}\right\}\right]^2\left.\right\}

+ (1 + \zeta^{-2}) \mathbb{E}_{t_\omega} \left[\left(\sum_{\ell=0}^{L-1} \partial_2 u(z_\ell, \ell + 1) \times\right.ight.

\times \left\{ \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i \omega \cdot z_\ell} d\omega dt - \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i \omega \cdot z_\ell} d\omega dt\right\}\right]^2.$$

To estimate the second expected value in the right hand side we will use that $\frac{dz_\ell}{dt}$ is small in the following sense. Lemma 4.1 implies that

$$\frac{dz_\ell}{dt} = \frac{f(x) - \beta(x)}{1 + \delta}$$

which is sufficiently small in order to obtain

$$\mathbb{E}_{t_\omega} \left[\left(\sum_{\ell=0}^{L-1} \partial_2 u(z_\ell, \ell + 1) \{\text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i \omega \cdot z_\ell} d\omega dt - \text{Re} \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i \omega \cdot z_\ell} d\omega dt\}\right)^2\right]$$

\leq \mathbb{E}_{t_\omega} \left[\left(\sum_{\ell=0}^{L-1} |\partial_2 u(z_\ell, \ell + 1)| \int_{t_\ell}^{t_{\ell+1}} \int_{\mathbb{R}} |\hat{b}(t, \omega)||\omega||z_\ell - z_\ell| d\omega dt\right)^2\right]

\leq \mathbb{E}_{t_\omega} \left[\left(\sum_{\ell=0}^{L-1} |\partial_2 u(z_\ell, \ell + 1)| \sup_t \int_{\mathbb{R}} |\hat{b}(t, \omega)||\omega||d\omega max(t_{\ell+1} - t_\ell) | f(x) - \beta(x) \right)^2\right]\frac{1}{1 + \delta}]

= O(L^{-2} K^{-1}).$

With $\beta = 0$ we would instead obtain the bound $O(L^{-2}).$
To estimate the first expected value in the right hand side of (5.17) we note that we have
\[ E_{t,\omega}[\text{Re} \sum_{k=1}^{K} \hat{c}_{ik} LKp'(t_{ik}, \omega_{ik}) e^{i\omega_{ik}x}] = \text{Re} \int_{t_{\ell}}^{t_{\ell+1}} \hat{c}(t, \omega) e^{i\omega x} d\omega dt \]
and by Lemma 3.1
\[ E_{t,\omega}[\left( \text{Re} \sum_{k=1}^{K} \frac{\hat{c}_{ik}}{LKp'(t_{ik}, \omega_{ik})} e^{i\omega_{ik}x} - \text{Re} \int_{t_{\ell}}^{t_{\ell+1}} \hat{c}(t, \omega) e^{i\omega x} d\omega dt \right)^2] = O(K^{-1}L^{-2}). \]
All terms
\[ \text{Re} \sum_{k=1}^{K} \frac{\hat{c}_{ik}}{LKp'(t_{ik}, \omega_{ik})} e^{i\omega_{ik}x} - \text{Re} \int_{t_{\ell}}^{t_{\ell+1}} \hat{c}(t, \omega) e^{i\omega x} d\omega dt \]
are independent for different \( \ell \), and \( \partial_{z} u(z_{\ell}) \) is deterministic. The zero mean and independence properties of terms in the first expected value in the right hand side of (5.17) imply
\[ E_{t,\omega}\left[ \left( \sum_{\ell=0}^{L-1} \partial_{z} u(z_{\ell}, \ell + 1) \{ \text{Re} \int_{t_{\ell}}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_{\ell}} d\omega dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{b}_{ik}}{LKp(t_{ik}, \omega_{ik})} e^{i\omega_{ik}z_{\ell}} \right) \right. \]
\[ + \left. \text{Re} \int_{t_{t}}^{t_{\ell+1}} \int_{\mathbb{R}^{d}} \hat{c}(t, \omega) e^{i\omega x} d\omega dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{c}_{ik}}{LKp'(t_{ik}, \omega_{ik})} e^{i\omega_{ik}x} \right)^2 \]
\[ = \sum_{\ell=0}^{L-1} E_{t,\omega}\left[ \left( \partial_{z} u(z_{\ell}, \ell + 1) \{ \text{Re} \int_{t_{\ell}}^{t_{\ell+1}} \int_{\mathbb{R}} \hat{b}(t, \omega) e^{i\omega z_{\ell}} d\omega dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{b}_{ik}}{LKp(t_{ik}, \omega_{ik})} e^{i\omega_{ik}z_{\ell}} \right) \right. \]
\[ + \left. \text{Re} \int_{t_{t}}^{t_{\ell+1}} \int_{\mathbb{R}^{d}} \hat{c}(t, \omega) e^{i\omega x} d\omega dt - \text{Re} \sum_{k=1}^{K} \frac{\hat{c}_{ik}}{LKp'(t_{ik}, \omega_{ik})} e^{i\omega_{ik}x} \right)^2 \].

The variance of these Monte Carlo approximations yields as in Lemma 3.1 and Lemma 4.2
\[ R_{0} = O(L^{-1}K^{-1} + L^{-4}), \]
where the constant in \( O(L^{-1}K^{-1}) \) is
\[ \int_{0}^{1} \int_{\mathbb{R}} \left| b(t, \omega) \right|^{2} \left| \partial_{z} u(z_{t}, t) \right|^{2} \frac{d\omega dt}{p(t, \omega)} + \int_{0}^{1} \int_{\mathbb{R}^{d}} \left| c(t, \omega) \right|^{2} \left| \partial_{z} u(z_{t}, t) \right|^{2} \frac{d\omega dt}{p'(t, \omega)}, \]
which by Lemma 3.2 becomes minimal for
\[ p(t, \omega) = \frac{\left| b(t, \omega) \right| \left| \partial_{z} u(z_{t}, t) \right|}{\int_{0}^{1} \int_{\mathbb{R}} \left| b(t, \omega) \right| \left| \partial_{z} u(z_{t}, t) \right| d\omega dt} \]
and
\[ p'(t, \omega) = \frac{\left| c(t, \omega) \right| \left| \partial_{z} u(z_{t}, t) \right|}{\int_{0}^{1} \int_{\mathbb{R}^{d}} \left| c(t, \omega) \right| \left| \partial_{z} u(z_{t}, t) \right| d\omega dt}. \]
Here we use the notation \( u(z, t) := z_{1} \) where \( z_{t} = z \) and \( z_{s} \) solves the differential equation constraint in (4.1) for \( s > t \).

For a deep residual neural network to be as accurate as a residual neural network with one hidden layer, asymptotically as \( LK \to \infty \), we therefore need
\[ \frac{1}{LK} + \frac{1}{K^{2}} + \frac{1}{L^{4}} \approx \frac{1}{LK} \]
which implies

\[ L \ll K \ll L^3, \]

and by choosing \( \zeta = \left( (\delta^2 + \epsilon^2)LK \right)^{1/2} \) in (5.1) we obtain (2.1). □

**Lemma 5.1** (Gronwall’s inequality). Assume there are positive constants \( \Gamma \) and \( \Lambda \) such that

\[ \eta_\ell \leq \Gamma \eta_{\ell-1} + \Lambda, \quad \ell = 1, 2, \ldots, L, \]

then

\[
\eta_\ell \leq \begin{cases} 
\Gamma^\ell \eta_0 + \Lambda \frac{\Gamma^{\ell-1}}{\Gamma-1}, & \Gamma \neq 1, \\
\eta_0 + \Lambda \ell, & \Gamma = 1.
\end{cases}
\]

**Proof.** The proof is well known and included here for completeness. We have

\[
\eta_\ell \leq \Gamma \eta_{\ell-1} + \Lambda \\
\leq \Gamma (\Gamma \eta_{\ell-2} + \Lambda) + \Lambda \\
= \Gamma^2 \eta_{\ell-2} + \Lambda (1 + \Gamma) \\
\leq \Gamma^2 (\Gamma \eta_{\ell-3} + \Lambda) + \Lambda (1 + \Gamma) \\
\leq \Gamma^3 \eta_{\ell-3} + \Lambda (1 + \Gamma + \Gamma^2) \\
\leq \Gamma^\ell \eta_0 + \Lambda (1 + \Gamma + \ldots + \Gamma^{\ell-1}) \\
= \begin{cases} 
\Gamma^\ell \eta_0 + \Lambda \frac{\Gamma^{\ell-1}}{\Gamma-1}, & \Gamma \neq 1, \\
\eta_0 + \Lambda \ell, & \Gamma = 1.
\end{cases}
\]

(5.18)

**Lemma 5.2** (Chernoff bound). Assume that \( \xi_j, j = 1, \ldots, J \) are independent identically distributed random variables on \( \mathbb{R} \) with mean zero, \( \mathbb{E}[\xi_1] = 0 \), and the exponential moment bound \( \mathbb{E}[e^{\theta \xi_1}] < \infty \), for \( \theta \) in a neighborhood of zero, then the probability for large deviations of the empirical mean has the exponential bound

\[
P(\left| \sum_{j=1}^J \xi_j \right| \geq \alpha) \leq e^{-JI(\alpha) + e^{-JI(-\alpha)}},
\]

where the Legendre transform \( I(\alpha) := \sup_{\theta \in \mathbb{R}} \theta \alpha - \log(\mathbb{E}[e^{\theta \xi_1}]) \) is positive for \( \alpha \in \mathbb{R} \setminus \{0\} \).

**Proof.** The proof is well known and included here for completeness. Taylor expansion implies

\[
I(\alpha) \geq \theta \alpha - \frac{\theta^2 \mathbb{E}[\xi_1^2]}{2} + o(\theta^2)
\]

so that \( I(\alpha) > 0 \) for \( \alpha \neq 0 \). We have for \( \theta \geq 0 \)

\[
P(\sum_{j=1}^J \xi_j \geq \alpha) = \mathbb{E}[1_{\{\sum_{j=1}^J \xi_j \geq J\alpha\}}] \\
\leq \mathbb{E}[e^{-\theta \alpha + \theta \sum_{j=1}^J \xi_j} 1_{\{\sum_{j=1}^J \xi_j \geq J\alpha\}}] \\
\leq e^{-\theta \alpha} \mathbb{E}[e^{\theta \sum_{j=1}^J \xi_j}] \\
= e^{-\theta \alpha} \left( \mathbb{E}[e^{\theta \xi_1}] \right)^J \\
= e^{-J(\theta \alpha - \log \mathbb{E}[e^{\theta \xi_1}])}.
\]

(5.20)
The estimate $P(\sum_{j=1}^{J} \xi_j \leq -\alpha) \leq e^{-J(\theta \alpha - \log E[e^{-\theta \xi_j}])}$ follows by applying (5.20) to $-\xi_j$ and we obtain (5.19) by maximizing with respect to $\theta \in \mathbb{R}$. \hfill \Box

6. Numerical algorithms

This section presents numerical algorithms based on the deep residual network optimization problem (1.10). First we motivate an explicit layer by layer method to approximate the deep residual network optimization problem (1.10) for given frequency distributions. This layer by layer method is then used in combination with an adaptive Metropolis random Fourier feature method to sample the frequencies in an optimal way, without explicit knowledge of the frequency distribution. The sampled frequencies with their corresponding amplitudes are then used as initial values to train the final residual network with a global optimizer.

6.1. A layer by layer approximation for amplitudes. Consider the problem with infinite number of layers and nodes in Lemma 4.1 and replace $f(x)$ by $y(x)$ and set $\beta(x) = 0$. As shown in (4.6), the Lagrange multiplier

$$\lambda_t(x) = 2(\tilde{z}_2(x) - y(x)),$$

is constant for each data point $x$ and layer $t$. We write the control as

$$\alpha(t, \tilde{z}_t(x), x) = \text{Re} \int_{\mathbb{R}} \hat{b}(t, \omega)e^{i\omega \tilde{z}_t(x)} d\omega + \text{Re} \int_{\mathbb{R}^d} \hat{c}(t, \omega)e^{i\omega' \cdot x} d\omega$$

$$= \text{Re}(S_b(x)\hat{b}(t, \cdot) + S_c(x)\hat{c}(t, \cdot))$$

and let

$$a(t, \cdot) := \begin{bmatrix} \hat{b}(t, \cdot) \\ \hat{c}(t, \cdot) \end{bmatrix},$$

$$S(x) := [S_b(x) \ S_c(x)],$$

so that $\alpha = \text{Re}(Sa)$. By the Pontryagin principle, the problem to determine the amplitudes $\hat{b}$ and $\hat{c}$ becomes

$$\arg \min_{\hat{b}(t, \cdot), \hat{c}(t, \cdot)} \mathbb{E}_{xy}[\lambda_t(x)\text{Re}(S(x)a) + \delta \left(\text{Re}(S(x)a)\right)^2]$$

$$= \arg \min_{\hat{b}(t, \cdot), \hat{c}(t, \cdot)} \mathbb{E}_{xy}[\frac{\lambda_t(x)}{\delta} \text{Re}(S(x)a) + \left(\text{Re}(S(x)a)\right)^2]$$

$$= \arg \min_{\hat{b}(t, \cdot), \hat{c}(t, \cdot)} \mathbb{E}_{xy}[\frac{\lambda_t(x)}{2\delta} + \text{Re}(S(x)a)]^2].$$

Based on a finite set of data $\{(x_n, y(x_n))\}_{n=1}^{N}$, the number of levels $L$ and nodes $K$, we assume that the residual is reduced by a factor $\delta$, from the levels $L$ to $\ell$ as

$$\frac{\lambda_t(x)}{2\delta} = \frac{2(\bar{z}_L(x) - y(x))}{2\delta} \approx \bar{z}_\ell(x) - y(x).$$
to obtain, by (6.1), the explicit layer by layer least squares approximation

\[
(\bar{b}_\ell, \bar{c}_\ell) = \arg\min_{\bar{b}_{\ell k} \in \mathbb{C}, \bar{c}_{\ell k} \in \mathbb{C}} \sum_{n=1}^{N} |z_\ell(x_n) + \text{Re}\left( \sum_{k=1}^{K} \bar{b}_{\ell k} e^{i\omega_{\ell k} z_\ell(x_n) + \sum_{k=1}^{K} \bar{c}_{\ell k} e^{i\omega'_{\ell k} x_n}) - y(x_n)|^2, \right.
\]

(6.2)

\[
z_{\ell+1}(x) = z_{\ell}(x) + \text{Re}\left( \sum_{k=1}^{K} \bar{b}_{\ell k} e^{i\omega_{\ell k} z_\ell(x)} + \sum_{k=1}^{K} \bar{c}_{\ell k} e^{i\omega'_{\ell k} x} \right), \quad \ell = 0, \ldots, L - 1,
\]

\[
z_0 = 0.
\]

6.2. **Layer by layer training of amplitudes and frequencies.** The goal of this section is to present Algorithm 2 that generalizes (6.2) to also adaptively sample the frequencies. The frequencies are updated by the Adaptive Metropolis sampling Algorithm 1, which asymptotically samples the optimal frequencies.

Algorithm 1 is introduced and described in detail in [8]. Algorithm 1 is based on the layer by layer method (6.2) with each least squares solution for the pre-training can be chosen significantly smaller than \( N \). When training layers deeper than the first hidden layer we use Algorithm 1 with a slight modification. The least squares problem defining the amplitudes is interchanged to the following least squares problem for the training data \( \{(x_n, y_n)\}_{n=1}^{N} \) the amplitudes are determined by linear least squares problems for the different frequencies updates

\[
\min_{\beta \in \mathbb{C}^K} (N^{-1}|S\hat{\beta} - y|^2 + \hat{\delta}|\hat{\beta}|^2),
\]

where \( S \in \mathbb{C}^{N \times K} \) is the matrix with elements \( S_{n,k} = e^{i\omega_{n,k} x_n} \), \( n = 1, \ldots, N \), \( k = 1, \ldots, K \) and \( y = (y_1, \ldots, y_N) \in \mathbb{R}^N \).

When training layers deeper than the first hidden layer we use Algorithm 1 with a slight modification. The least squares problem defining the amplitudes is interchanged to the following least squares problem for the training data \( \{(x_n, y_n)\}_{n=1}^{N} \),

\[
\min_{\bar{c}, \bar{b} \in \mathbb{C}^K} (N^{-1}|S \begin{bmatrix} \bar{c} \\ \bar{b} \end{bmatrix} - y|^2 + \hat{\delta}|(\bar{c}, \bar{b})|^2),
\]

where \( S \in \mathbb{C}^{N \times 2K} \) is the matrix with elements \( S_{n,k} = e^{i\omega_{n,k} z_\ell(x_n)} \) for \( n = 1, \ldots, N \), \( k = 1, \ldots, K \), and \( S_{n,k} = e^{i\omega_{n,k} z_\ell(x_n)} \) for \( n = 1, \ldots, N \), \( k = K + 1, \ldots, 2K \) and \( y = (y_1, \ldots, y_N) \in \mathbb{R}^N \). The frequencies \( \omega_{\ell k} \) are samples from the standard normal distribution and they are never updated.

Algorithm 2 is based on the layer by layer method (6.2) with each least squares solution replaced by calling adaptive the Metropolis Algorithm 1. When running Algorithm 1 with the modification (6.4) used in Algorithm 2 we say that we run the modified Algorithm 1.

In the layer by layer method (6.2) the first layer starting with \( z_0 = 0 \) will precisely do the initial step of constructing \( \beta \) in (1.8), (1.9) and (1.10). Therefore Algorithms 2 and 3 are formulated without mentioning \( \beta \).

6.3. **Global post-training.** In the layer by layer build up of a residual neural network each layer is optimized at a time. As post-training after running Algorithm 2 a global optimizer, training the whole residual network, is used to further increase the approximation property of the residual neural network as presented in Algorithm 3. In Algorithm 3 the choice of the number of training points \( N_\ell \) for the pre-training can be chosen significantly smaller than \( N \) according to our experimental results.
Algorithm 1 Adaptive random Fourier features with Metropolis sampling

Input: \( \{(x_n, y_n)\}_{n=1}^{N} \{\text{data}\} \)
Output: \( x \mapsto \sum_{k=1}^{K} \hat{\beta}_k e^{i\omega_k \cdot x} \{\text{random features}\} \)
Choose a sampling time \( T \), a proposal step length \( \delta \), an exponent \( \gamma \), a Tikhonov parameter \( \hat{\delta} \) and a frequency \( m \) of \( \hat{\beta} \) updates

\[
\begin{align*}
M & \leftarrow \text{integer part } (T/\delta^2) \\
\omega & \leftarrow \text{the zero vector in } \mathbb{R}^{Kd} \\
\hat{\beta} & \leftarrow \text{minimizer of the problem } (6.3) \text{ given } \omega \\
\text{for } i = 1 \text{ to } M \text{ do} \\
\quad r_N & \leftarrow \text{standard normal random vector in } \mathbb{R}^{Kd} \\
\quad \omega' & \leftarrow \omega + \delta r_N \{\text{random walk Metropolis proposal}\} \\
\quad \hat{\beta}' & \leftarrow \text{minimizer of the problem } (6.3) \text{ given } \omega' \\
\text{for } k = 1 \text{ to } K \text{ do} \\
\quad r_U & \leftarrow \text{sample from uniform distribution on } [0, 1] \\
\quad \text{if } |\hat{\beta}'_k|^\gamma / |\hat{\beta}_k|^\gamma > r_U \{\text{Metropolis test}\} \text{ then} \\
\quad \quad \omega_k & \leftarrow \omega'_k \\
\quad \quad \hat{\beta}_k & \leftarrow \hat{\beta}'_k \\
\quad \text{end if} \\
\text{end for} \\
\text{if } i \mod m = 0 \text{ then} \\
\quad \hat{\beta} & \leftarrow \text{minimizer of the problem } (6.3) \text{ with adaptive } \omega \\
\text{end if} \\
\text{end for} \\
\hat{\beta} & \leftarrow \text{minimizer of the problem } (6.3) \text{ with adaptive } \omega \\
x & \mapsto \sum_{k=1}^{K} \hat{\beta}_k e^{i\omega_k \cdot x} 
\end{align*}
\]

Algorithm 2 Layer by layer adaptive random Fourier features with Metropolis sampling

Input: \( \{(x_n, y_n)\}_{n=1}^{N} \{\text{data}\} \)
Output: \( x \mapsto \bar{z}_L(x) \{\text{Residual network}\} \)
Choose the number of layers \( L \)

\[
\begin{align*}
\bar{z}_1 & \leftarrow \text{real part of output from Algorithm } 1 \text{ run on data } \{(x_n, y_n)\}_{n=1}^{N} \\
\{r_n\}_{n=1}^{N} & \leftarrow \{y_n - \bar{z}_1(x_n)\}_{n=1}^{N} \\
\text{for } \ell = 2 \text{ to } L \text{ do} \\
\quad S_a & \leftarrow \text{real part of output from modified Algorithm } 1 \text{ run on data } \{(x_n, r_n)\}_{n=1}^{N} \\
\quad \bar{z}_\ell & = \bar{z}_{\ell-1} + S_a \\
\quad \{r_n\}_{n=1}^{N} & \leftarrow \{y_n - \bar{z}_\ell(x_n)\}_{n=1}^{N} \\
\text{end for} \\
x & \mapsto \bar{z}_L(x)
\end{align*}
\]

7. Numerical experiments

In this section we present numerical experiments. A purpose is to study how the generalization error behaves in practice with respect to the total number of nodes \( LK \). Another purpose is to study how the generalization error depends on the choice of algorithm to train the residual neural network. This is done with three methods:
Algorithm 3 Global optimization of layer by layer pre-trained residual network

Input: \{ (x_n, y_n) \}_{n=1}^{N} \{ data \}
Output: \( x \mapsto \bar{z}_L(x) \) \{ Residual network \}

Choose the number of layers \( L \) and the number of data points \( N_1 \leq N \) for the pre-training

\[
\begin{align*}
\bar{z}_L &\leftarrow \text{output from Algorithm 2 run on data } \{ (x_n, y_n) \}_{n=1}^{N_1} \\
\bar{z}_L &\leftarrow \text{output from global optimizer run on } \bar{z}_L \text{ and data } \{ (x_n, y_n) \}_{n=1}^{N} \\
x &\mapsto \bar{z}_L(x)
\end{align*}
\]

- Method 1: The residual networks are trained by Algorithm 2
- Method 2: The residual networks are trained by a global optimizer.
- Method 3: The residual networks are trained by Algorithm 3

Consider the target functions

\[
f_1(x) = \text{Si} \left( \frac{x_1}{a} \right) e^{-|x|^2/2}
\]
and

\[
f_2(x) = \text{Si} \left( \frac{x_1}{a} \right) e^{-|x_1|^2/2}
\]

where \( a = 10^{-2} \) and

\[
\text{Si}(v) := \int_0^v \frac{\sin(t)}{t} dt
\]
is the so called Sine integral. We generate training data by sampling the components of \( x_n = (x_{n1}, x_{n2}, \ldots, x_{nd}) \in \mathbb{R}^d \) from the standard normal distribution, setting \( y_n = f_1(x_n) \) or \( y_n = f_2(x_n) \) and normalizing the data by subtracting the mean and dividing by the standard deviation component wise. The test data is generated analogously but normalized with the mean and the standard deviation computed from the training data set. The parameter choices are presented in Table 2. For Method 1, error bars are generated and presented in Figure 2. The error bars are defined as the closed intervals

\[
[e_K - 2\sigma_K, e_K + 2\sigma_K]
\]

where \( \sigma_K \) is the empirical standard deviation of the generalization error and \( e_K \) is the empirical mean of the generalization errors after \( \bar{M} \) independent realizations.

When running Method 3 we generate Figure 6 where instead of error bars we present 11 outcomes for each \( LK \) when \( L = 1 \) and 10 outcomes for each \( LK \) when \( L = 5 \).

7.1. Method 1: The residual networks are trained by Algorithm 2. With Method 1 we build up the residual neural network layer by layer with Algorithm 2. The number of iterations per layer, in Algorithm 1, is chosen large with the purpose of minimizing the error. In Figure 2 the generalization error, with error bars, with respect to \( LK \) is presented for two different values of \( L \).

7.2. Method 2: The residual networks are trained by a global optimizer. In Method 2 we run the global optimizer ADAM, see [9], with frequencies and amplitudes initialized by Xavier normal initialization, see [6], with a learning rate decreasing as \( \Delta t_e/t_e \) where \( \Delta t_e \) is the initial learning rate and \( t_e \) is epoch number \( t_e \). The fact that the choice of initial distribution of the frequencies and amplitudes is not obvious in all situations is partly a motivation for Algorithm 3 which, with Algorithm 2 assymptotically samples the optimal
7.3. The residual networks are trained by Algorithm 3. With Method 3 we run Algorithm 3. That is, we build up a residual neural network layer by layer which we use as an initial neural network for a global optimizer. In this case we choose ADAM with decreasing learning rate, as with Method 2, as the global optimizer.

The main purpose of Method 3 is to study how the generalization error depends on $LK$ and in Figure 6 we can see how the generalization error depends on $LK$. In Figures 3 and 4 we present the neural network plotted and in Table 1 we can see the empirical average of the generalization errors and the standard deviation after $\bar{M}$ independent runs.

7.4. Summary of experimental results. In Table 1 we see that Method 3, i.e. Layer by layer & ADAM, produces a smaller value of the generalization error than Method 2 does, i.e. ADAM initialized by Xavier, for the chosen number of epochs for both target functions $f_1$ and $f_2$. We note from Figure 3 that the approximation Method 3 produces is a better fit to the target function than Method 2 produces. Both methods would give better results for larger values of $K$ and if ran for a larger number of epochs. It can not be concluded that Method 2 eventually would not produce a generalization error of approximately the same value as Method 3 does.
Figure 2. The figure illustrates for Method 1 the generalization error, with error bars defined as (7.1), with respect to the total number of nodes, \( LK \), for a target function in dimension \( d = 3 \). Three cases are presented: errors for a one layer neural network, errors for a five layer neural network and errors for a five layer neural network where \( \bar{z}_{\ell+1} - \bar{z}_\ell \) is defined to be a one layer neural network with frequencies in dimension \( d + 1 \) and data for \( L > 1 \) is on the form \( \{(x_n, \hat{z}_{\ell}(x_n)), y_n\}_{n=1}^N \).

In Figure 2 the generalization error decreases as expected as \( \mathcal{O}((LK)^{-1}) \) and we note that for a fixed value of \( LK \), the generalization error in Method 1 is, also as expected, smaller for \( L = 5 \) than for \( L = 1 \).

Figure 5 shows how the error decreases with respect to the number of epochs for ADAM iterations. At that specific run the number of epochs is chosen to 100 with the purpose to limit the computation time even though the error continues to decrease. The choice of the number of epochs to run is a balance between getting the smallest error and getting a reasonable computation time.

When running Method 3 for several independent instances and several different values of \( LK \) we note, from Figure 6, that when \( L = 1 \) the generalization error has much smaller spread between each instance compared to when \( L = 5 \). On the other hand, the generalization error is much smaller for each run when \( L = 5 \) than when \( L = 1 \).
Figure 3. Target function $f_1$ and approximating neural network are presented where the subfigures to the left show a slice of the functions along the $x_1$-axis and the figures to the right shows the function values plotted against the target function values. The problem is in dimension $d = 10$.

8. Conclusions

A mean field optimal control applied to deep residual networks based on random Fourier features is used to derive an optimal distribution of random Fourier features. This provides smaller generalization error compared to the well known estimate by Barron for a network with one hidden layer and the same total number of nodes. The insight provided by this result is used to construct a new layer by layer training algorithm. The layer by layer method samples the optimal distribution using an adaptive Metropolis method, where the computed amplitudes are used in the Metropolis proposal step. The layer by layer method is used as an initialization for a global optimizer, such as ADAM.
(a) Method 2: Xavier & ADAM

(b) Method 2: Xavier & ADAM

(c) Method 3: Layer by layer & ADAM

(d) Method 3: Layer by layer & ADAM

**Figure 4.** Target function $f_2$ and approximating neural network are presented where the subfigures to the left show all the function values along the $x_1$-axis and the figures to the right show the function values plotted against the target function values. The problem is in dimension $d = 10$. For Method 3, Layer by Layer & ADAM, the neural network values are under the target function values.

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Figure 5. The TensorBoard, see [http://tensorflow.org/tensorboard/](http://tensorflow.org/tensorboard/) generated figure shows how the training error (orange) and the validation error (blue) decreases with respect to the number of epochs when running Method 2.

| Method | Regression |
|--------|------------|
| Algorithm | Algorithm 2 | Xavier + ADAM | Algorithm 3 |
| $d$ | 3 | 10 | 4 | 10 | 10 |
| $LK$ | $5 \times 2^i$, $i = 1, 2, ..., 6$ | 2560 | 1280 | $5 \times 2^i$, $i = 1, 2, ..., 8$ | 2560 | 1280 |
| $L$ | 1 and 5 | 10 | 1 | 5 | 10 |
| $N$ | $2 \times 10^4$ | 10$^6$ |
| $N$ | $2 \times 10^4$ | 10$^6$ |
| Target function | $f_1$, $f_2$, $f_1$, $f_2$ |
| $N_1$ | | | | $10^4$ |
| $M$ | 10 | 20 | 11 | 10 | 10 | 10 |
| $\gamma$ | $3d - 2$ | | $3d - 2$ |
| $\delta$ | 1.1 | | 1.1 |
| $M$ | 2000 | 200 | 400 | 600 |
| Batch size | 100 |
| Number of epochs | 100 | 200 | 150 | 100 | 200 |
| $\delta$ | $0.5 \times 2.4^2/d$ | | $0.5 \times 2.4^2/d$ |
| $\Delta t_e$ | | | | 0.001 |
| $m$ | 1 | 3c 3d 3e 4d | 3c 3d 4c 4d |
| Table | 1 | 1 |

Table 2. Summary of the parameter choices for the numerical experiments.

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Figure 6. The figure illustrates how the generalization error depends on the total number of nodes, $L K$, in Method 3. For each value of $L K$ the 11 blue dots and the 10 red dots shows the different outcomes of the generalization error for $L = 1$ and $L = 5$ respectively. The blue dots are almost on top of each other. The problem is in dimension $d = 4$.

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KTH Royal Institute of Technology, Stockholm, Sweden

RWTH Aachen University, Aachen, Germany and KTH Royal Institute of Technology, Stockholm, Sweden

University of Delaware, Newark, USA,

KTH Royal Institute of Technology, Stockholm, Sweden

KTH Royal Institute of Technology, Stockholm, Sweden

RWTH Aachen University, Aachen, Germany and KAUST, Saudi Arabia