A type of generalization error induced by initialization in deep neural networks

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Abstract

How different initializations and loss functions affect the learning of a deep neural network (DNN), specifically its generalization error, is an important problem in practice. In this work, focusing on regression problems, we develop a kernel-norm minimization framework for the analysis of DNNs in the kernel regime in which the number of neurons in each hidden layer is sufficiently large (Jacot et al. 2018, Lee et al. 2019). We find that, in the kernel regime, for any loss in a general class of functions, e.g., any $L^p$ loss for $1 < p < \infty$, the DNN finds the same global minima—the one that is nearest to the initial value in the parameter space, or equivalently, the one that is closest to the initial DNN output in the corresponding reproducing kernel Hilbert space. With this framework, we prove that a non-zero initial output increases the generalization error of DNN. We further propose an antisymmetrical initialization (ASI) trick that eliminates this type of error and accelerates the training. We also demonstrate experimentally that even for DNNs in the non-kernel regime, our theoretical analysis and the ASI trick remain effective. Overall, our work provides insight into how initialization and loss function quantitatively affect the generalization of DNNs, and also provides guidance for the training of DNNs.

1 Introduction

The wide application of deep learning makes it increasingly urgent to establish quantitative theoretical understanding of the learning and generalization behaviors of deep neural networks (DNNs). In this work, we study theoretically the problem of how initialization and loss function quantitatively affect these behaviors of DNNs. Our study focuses on the regression problem, which plays a key role in many applications, e.g., simulation of physical systems (Zhang et al. 2018), prediction of time series (Qiu et al. 2014) and solving differential equations (E & Yu 2018, Xu et al. 2019). For theoretical analysis, we consider an extremely over-parameterized regime of DNN, i.e., number of neurons in each layer tends to infinity, which has attracted significant attentions recently. In this
regime, the training dynamics of a DNN is found to be well approximated by the gradient flow of a linearized model of the DNN resembling kernel methods (Jacot et al. 2018, Lee et al. 2019). In our work, we refer to the regime of DNNs with this property as the kernel regime and we do not distinguish “linearized model of DNN” and “DNN in the kernel regime” for the analysis of their properties. Note that, theoretical investigation of such a regime can provide insight into the understanding of general DNNs in practice by the following facts. Heavy overparameterization is one of the key empirical tricks to overcome the learning difficulty of DNNs (Zhang et al. 2016). The DNNs in extremely over-parameterized regime preserve substantive behavior as those in mildly over-parameterized regime. For example, stochastic gradient descent (SGD) can find global minima of the training objective of DNNs which generalizes well to the unseen data (Zhang et al. 2016).

In general, the error of DNN can be classified into three general types (Poggio et al. 2018): approximation error induced by the capacity of the hypothesis set, generalization error induced by the given training data, and training error induced by the given training algorithm. By the universal approximation theorem (Cybenko 1989) and empirical experiments (Zhang et al. 2016), a large neural network often has the power to express functions of real datasets (small approximation error) and the gradient-based training often can find global minima (zero training error). Therefore, generalization error is the main source of error in applications. It can be affected by many factors, such as initialization and loss function as widely observed in experiments. Empirically, a large weight initialization often leads to a large generalization error (Xu et al. 2018, 2019). However, a too small weight initialization makes the training extremely slow. Note that zero initialization leads to a saddle point of DNN which makes the training impossible. Despite above empirically observations, it remains unclear how initialization is related to the generalization error. Regarding the loss function, it is also unclear how it affects the behavior of DNNs.

Our contribution is concluded as follows. Focusing on the regression problem, we develop a kernel-norm minimization framework for the analysis of DNNs in the kernel regime based on the following theoretical results.

i) We prove that, for a general class of loss functions, e.g., any $L^p$ loss for $1 < p < \infty$, the gradient flow of DNN in the kernel regime, despite trajectory difference, finds the same global minimum.

ii) Similar to Mei et al. (2019), we prove that, among the huge set of all global minima, this global minimum is the nearest to the initial value in the parameter space, or equivalently, is the closest to the initial DNN output $h_{\text{ini}}$ in the corresponding reproducing kernel Hilbert space (RKHS).

With the above framework, we analyze theoretically the impact of a non-zero initial DNN output $h_{\text{ini}}$.

i) We quantify how a $h_{\text{ini}}$ affects the solution of the kernel-norm minimization problem.

ii) We prove that a random $h_{\text{ini}}$ leads to a specific type of generalization error.

iii) We propose an AntiSymmetrical Initialization (ASI) trick which eliminates this generalization error and accelerates training while keeping the kernel of DNN unchanged.

Experimentally, we demonstrate that our theory accurately predicts the behavior of wide DNNs. Moreover, we demonstrate that the ASI trick remains effective for DNNs in the non-kernel regime as well as for the classification problem.

2 Related works

There are a series of works following the study of Jacot et al. (2018) on the kernel regime. For example, theoretical works provide insight into how SGD can find global minima on the training objective of DNNs (Du et al. 2018, Zou et al. 2018) and how fast the training can be done (Allen-Zhu et al. 2018, E, Ma, Wang & Wu 2019, E, Ma & Wu 2019). The generalization error bounds (Arora et al. 2019, Cao & Gu 2019, E, Ma, Wang & Wu 2019, E, Ma & Wu 2019) are further studied in the kernel regime. In addition, the type of generalization error that vanishes as the width of DNN increases is analyzed (Geiger et al. 2019). Mei et al. (2019), Banburski et al. (2019) also found that the learning of DNNs in the kernel regime is associated with an optimization problem, however, they only consider the loss of mean-squared error (MSE) and a special initialization.
Chizat & Bach (2018) shows that if the initial DNN output is close enough to 0 and a large factor is used to scale the DNN output, the DNN with MSE loss selects parameters that are close to the initialization. Oymak & Soltanolkotabi (2018), Jacot et al. (2018) show that in an over-parameterized regime, the convergence point in the parameter space of a DNN remains close to the initialization. However, it remains unclear that, among all global optima of the loss, whether the gradient descent (GD) algorithm converges to one with the nearest distance to the initialization.

Previous works (Xu et al. 2018, Xu 2018, Xu et al. 2019, Rahaman et al. 2018) discover a Frequency-Principle (F-Principle) that DNNs prefer to learn the training data by a low-frequency function. Based on F-principle, Xu et al. (2018, 2019) point out that the final output of a DNN tends to inherit high frequencies of its initial output that can not be well constrained by the training data (Xu et al. 2018, 2019). Note that this understanding is consistent with our quantitative study.

3 Preliminary

A summary of notations can be found in Appendix 9.

3.1 Kernel regime of DNN

In the following, we consider the regression problem of fitting the target function \( f \in L^p(\Omega) \), where \( \Omega \) is a compact domain in \( \mathbb{R}^N \). Clearly, \( f \in L^p(\Omega) \) for \( 1 \leq p \leq \infty \). Specifically, we use a DNN, \( h_{DNN}(x, \theta(t)) : \Omega \times \mathbb{R}^{NP} \rightarrow \mathbb{R} \), to fit the training dataset \( \{x_i; y_i\}_{i=1}^M \) of \( M \) sampling points, where \( x_i \in \Omega \), \( y_i = f(x_i) \) for each \( i \). For the convenience of notation, we denote \( X = [x_1, \cdots, x_M]^T \), \( Y = [y_1, \cdots, y_M]^T \), and \( g(X) := [g(x_1), \cdots, g(x_M)]^T \) for any function \( g \) defined on \( \Omega \). It has been shown in Jacot et al. (2018), Lee et al. (2019) that, for any \( t \geq 0 \), if the number of neurons in each hidden layer is sufficiently large, then \( |\theta(t) - \theta(0)| \ll 1 \). In such cases, the following linearized model

\[
h(x, \theta) = h_{DNN}(x, \theta_0) + \nabla_\theta h_{DNN}(x, \theta_0)(\theta - \theta_0).
\]

is a very good approximation of DNN output \( h_{DNN}(x, \theta_{DNN}(t)) \) initialized with \( \theta_{DNN}(0) = \theta_0 \). Note that, we have the following requirements for \( h_{DNN} \) which are easily satisfied for common DNNs: For any \( \theta \in \mathbb{R}^{NP} \), there exists a weak derivative of \( h_{DNN}(\cdot, \theta) \) with respect to \( \theta \) and \( \nabla_\theta h_{DNN}(\cdot, \theta) \in L^2(\Omega) \). For the loss function

\[
L(\theta) = D(h(X, \theta), Y),
\]

where \( D \) is the distance function to be explained in Section 4, the gradient flow of \( \theta(t) \) with respect to the linearized model \( h(x, \theta(t)) \) follows

\[
\frac{d\theta(t)}{dt} = -\nabla_\theta h(x, \theta_0)^T \nabla_{h(x, \theta_0)} D(h(x, \theta(t)), Y),
\]

with initial value \( \theta(0) = \theta_0 \), where \( \nabla_\theta h(x, \theta_0) \in \mathbb{R}^{M \times NP}, \{\nabla_\theta h(x, \theta_0)\}_{ij} = \nabla_{x_j} h(x_i, \theta_0), \nabla_{h(x, \theta_0)} D(h(X, \theta(t)), Y) \in \mathbb{R}^M \). We refer to the regime in which \( h(x, \theta(t)) \) well approximate \( h_{DNN}(x, \theta_{DNN}(t)) \) under the same loss initialized by \( \theta_{DNN}(0) = \theta_0 \) for any \( t \geq 0 \) as the kernel regime of DNN. Therefore, in the following, our analysis focuses on dynamics (2) for the analysis of the behavior of DNN in the kernel regime. Eq. (1) yields the following dynamics of \( h(x, t) = h(x, \theta(t)) \),

\[
\partial_t h(x, t) = -K(x, X)\nabla_{h(x, t)} D(h(x, t), Y),
\]

with initial value \( h(\cdot, 0) = h(\cdot, \theta_0) \), where the kernel \( K \) is defined as

\[
K(\cdot, \cdot) = \nabla_\theta h(\cdot, \theta_0)|\nabla_\theta h(\cdot, \theta_0)^T,
\]

\( \nabla_\theta h(\cdot, \theta_0) = [\partial_{\theta_1} h(\cdot, \theta_0), \cdots, \partial_{\theta_{NP}} h(\cdot, \theta_0)] \) \( K(x, X) \in \mathbb{R}^{1 \times M} \) for any \( x \in \Omega \). Note that Eq. (3) of \( h \) is a closed system. By Jacot et al. (2018), \( K \) is symmetric and positive semi-definite. In the following, we may denote \( K_{h0}(\cdot, \cdot) = \nabla_\theta h(\cdot, \theta_0)|\nabla_\theta h(\cdot, \theta_0)^T \) when we need to differentiate kernels corresponding to different architectures or different initializations of DNNs.

3.2 Reproducing kernel Hilbert space (RKHS)

The kernel \( K \) can induce a RKHS as follows. First, we cite the Mercer’s theorem (Mercer (1909)).
We consider the gradient flow under any loss \( L \) where
\[
\langle \cdot \rangle = \int_{\Omega} K(\cdot, x) g(x) \, dx
\]
such that the corresponding sequence of eigenvalues \( \sigma_j \) is nonnegative. The eigenfunctions corresponding to non-zero eigenvalues are continuous on \( \Omega \) and \( K \) has the representation
\[
K(x, y) = \sum_{j=1}^{\infty} \sigma_j \phi_j(x) \phi_j(y),
\]
where the convergence is absolute and uniform.

Then, we can define the RKHS as \( \mathcal{H}_K(\Omega) := \{ g \in L^2(\Omega) \mid \sum_{i=1}^{\infty} \sigma_i^{-1} \langle g, \phi_i \rangle^2_{L^2(\Omega)} < \infty \} \), and the inner product in \( \mathcal{H}_K(\Omega) \) is given by
\[
\langle f, g \rangle_K = \sum_{i=1}^{\infty} \sigma_i^{-1} \langle f, \phi_i \rangle_{L^2(\Omega)} \langle g, \phi_i \rangle_{L^2(\Omega)},
\]
where \( \langle g, \phi_i \rangle_{L^2(\Omega)} = \int_{\Omega} g(x) \phi_i(x) \, dx \). Define \( K^{-1}(x, x') = \sum_{i=1}^{\infty} \sigma_i \phi_i(x) \phi_i(x') \), then the kernel norm of any \( g \in \mathcal{H}_K(\Omega) \) can be expressed as
\[
\|g\|_K = \langle g, g \rangle_K^{1/2} = \left( \int_{\Omega} g(x) g(x') K^{-1}(x, x') \, dx \, dx' \right)^{1/2}.
\]
\( \mathcal{H}_K(\Omega) \) satisfies [Berlinet & Thomas-Agnan, 2004]: (i) \( \forall x \in \Omega, K(\cdot, x) \in \mathcal{H}_K(\Omega) \); (ii) \( \forall x \in \Omega, \forall f \in \mathcal{H}_K, \langle f(\cdot), K(\cdot, x) \rangle_K = f(x) \); (iii) \( \forall x, y \in \Omega, (K(\cdot, x), K(\cdot, y))_K = K(x, y) \).

## 4 Kernel-norm minimization framework for DNNs in the kernel regime

In this section, we introduce the kernel-norm minimization framework for the analysis of DNNs in kernel regime. As introduced in Section 3.1, for the analysis of gradient flow of \( h_{\text{DNN}}(\cdot, \theta_{\text{DNN}}(t)) \) in the kernel regime, we focus on the gradient flow of its linearized model \( h(\cdot, \theta(t)) \), i.e., Eqs. (2), (5).

We consider the gradient flow under any loss \( L(\theta) = D(h(X, \theta), Y) \), where \( D \) is continuously differentiable and satisfies, for any \( z \in \mathbb{R}^M \), (i) \( D(z, z) = 0 \); (ii) \( D(z', z) \) attains minimum if and only if \( z' = z \). (iii) \( z' = z \) if and only if \( \nabla_z D(z', z) = 0 \). For example, \( D(h(X, \theta), Y) = \frac{1}{M} \sum_{i=1}^{M} |h(x_i, \theta) - y_i|^p \) for any \( 1 < p < \infty \). By Theorem 5 in Appendix 10, the long time solution \( \theta(\infty) = \lim_{t \to \infty} \theta(t) \) of dynamics (2) is equivalent to the solution of the optimization problem
\[
\min_{\theta} \|\theta - \theta_0\|_2, \quad \text{s.t.}, \quad h(X, \theta) = Y.
\]
By Theorem 8 in Appendix 10, \( h(x, \theta(\infty)) \) uniquely solves the optimization problem
\[
\min_{h-h_{\text{lin}} \in \mathcal{H}_K(\Omega)} \|h-h_{\text{lin}}\|_K, \quad \text{s.t.}, \quad h(X) = Y,
\]
where \( h_{\text{lin}}(x) = h(x, \theta_0) \) and the constraints \( h(X) = Y \) are in the sense of trace [Evans, 2010, pp. 257–261]. The above results hold for any initial value \( \theta_0 \). We refer to kernel-norm minimization framework as using the optimization problem (2) or (5) to analyze the long time solution of gradient flow dynamics (2) or (5), respectively.

With this framework, we emphasize the following results. First, for a finite set of training data, given \( \theta_0 \), because \( D \) is absent in problems (2) and (5), the output function of a well-trained DNN in the kernel regime is invariant to different choices of loss functions. Note that this result is surprising in the sense that different \( D \) clearly leads to different trajectories of \( \theta(t) \) and \( h(\cdot, \theta(t)) \). Based on this result, it is not necessary to stick to commonly used MSE loss for regression problems. For example, in practice, one can use \( D(h(X, \theta), Y) = \frac{1}{M} \sum_{i=1}^{M} |h(x_i, \theta) - y_i|^p \) of \( 1 < p < 2 \) to accelerate the training of DNN near convergence or \( 2 < p < \infty \) to accelerate the training near initialization. One can even mixing different loss functions to further boost the training speed. Second, among all sets of parameters that fit the training data, a DNN in the kernel regime always finds the one closest to the initialization in the parameter space with respect to the \( L^2 \) norm. Third, in the functional space, this framework shows that DNNs always seek to learn a function that has a shortest distance (with respect to the kernel norm) to the initial output function. In the following, we denote \( h_K(x; h_{\text{lin}}, X, Y) \) as the solution of problem (5) depending on \( K, h_{\text{lin}}, X \) and \( Y \).
5 Impact of non-zero initial output

Problems (4) and (5) explicitly incorporate the effect of initialization, thus enabling us to study quantitatively its impact to the learning of DNNs. In this section, we use the above framework to show that a random non-zero initial DNN output leads to a specific type of generalization error. We begin with a relation between the solution with zero initial output and that with non-zero initial output. Proofs of the following theorems can be found in Appendix [11]

Theorem 2. For a fixed kernel function \( K \in L^2(\Omega \times \Omega) \), and training set \( \{X;Y\} \), for any initial function \( h_{ini} \in L^\infty(\Omega) \), \( h_K(\cdot;h_{ini},X,Y) \) can be decomposed as

\[
h_K(\cdot;h_{ini},X,Y) = h_K(\cdot;0,X,Y) + h_{ini} - h_K(\cdot;0,X,h_{ini}(X)).
\] (6)

This theorem unravels the positive impact of a nonzero initialization, i.e., \( h_{ini} \neq 0 \), to the output function of a well-trained DNN in the kernel regime. Comparing the dynamics in (3) of zero and non-zero initialization, at the beginning, the difference of DNN output is \( h_{ini} \), whereas, at the end of the training, that difference shrinks to \( h_{ini} - h_K(\cdot;0,X,h_{ini}(X)) \), which is the residual of fitting \( h_{ini} \) sampled at \( X \) by the same DNN. Note that Geiger et al. [2019] figures out qualitatively that \( h_{ini} \), which does not vanish as the width of DNN tends to infinity, decreases during the training. However, they do not arrive at a quantitative relation as revealed by Theorem 2.

The expected generalization error of DNN with a random non-zero initial output can be estimated as follows.

Theorem 3. For a target function \( f \in L^\infty(\Omega) \), if \( h_{ini} \) is generated from an unbiased random function distribution \( P \) such that \( \mathbb{E}_{h_{ini} \sim P}h_{ini} = 0 \), then the generalization error of \( h_K(\cdot;h_{ini},X,f(X)) \) can be decomposed as follows

\[
\mathbb{E}_{h_{ini} \sim P}(h_K(\cdot;h_{ini},X,f(X),f)) = L(h_K(\cdot;0,X,f(X),f)) + \mathbb{E}_{h_{ini} \sim P}(h_M(\cdot;0,X,h_{ini}(X)),h_{ini}), \tag{7}
\]

where \( L(h_K(\cdot;h_{ini},X,f(X),f)) = ||h_K(\cdot;h_{ini},X,f(X)) - f||^2_{L^2(\Omega)} \).

By above theorem, \( \mathbb{E}_{h_{ini} \sim P}(h_M(\cdot;0,X,h_{ini}(X)),h_{ini}) \geq 0 \) is a specific type of generalization error induced by \( h_{ini} \). Clearly, this error decreases as the sample size \( M \) increases and as \( M \to \infty \), \( h_{ini} - h_K(\cdot;0,X,h_{ini}(X)) \to 0 \), which conforms with our intuition that if the optimization is sufficiently constrained by the training data, then the effect of initialization can be ignored. For real datasets of a limited number of training samples, this error is in general non-zero. By F-Principle [Xu et al., 2018], DNNs tend to fit training data by low frequency functions. Therefore, qualitatively, \( h_{ini} - h_K(\cdot;0,X,h_{ini}(X)) \) consists mainly of the high frequencies of \( h_{ini} \) which cannot be well constrained at \( X \).

6 AntiSymmetrical Initialization trick (ASI)

In general, from the Bayesian inference perspective, for fixed \( K \), a random \( h_{ini} \) introduces a prior to the inference that is irrelevant to the target function, thus should lower the accuracy of inference. To eliminate the negative impact of non-zero initial DNN output, a naive way is to set the initial output of the \( i \)th node of the \( l \)th layer of a DNN to zero but also keep the kernel invariant. Let \( h_{ini}^{[l]} \) be the output of the \( i \)th node of the \( l \)th layer of a DNN with \( h_{ini}^{[l]}(x) = 0 \). Then, \( h_l(x) = \theta^T(W_l^{[l]}h^{[l-1]}(x) + b_l^{[l]}) \), for \( i = 1, \ldots, \Theta \). After initializing the DNN by any method, we obtain \( h_i^{[H]}(x,\theta(0)) = [W_i^{[H]}(0), b_i^{[H]}(0), W_i^{[H-1]}(0), b_i^{[H-1]}(0), \ldots, b_i^{[1]}(0)] \).

The ASI for general loss functions is to consider a new DNN expressed as \( h_{ASI}(x,\Theta(t)) = \frac{\sqrt{\pi}}{\pi} h_i^{[H]}(x,\theta(t)) - \frac{\sqrt{\pi}}{\pi} h_i^{[H]}(x,\theta'()) \) where \( \Theta = [0,\theta'] \). \( \Theta \) is initialized such that \( \theta'(0) = \theta(0) \). In the following, we prove a theorem that ASI trick eliminates the nonzero random prior without changing the kernel \( K \). (Proof can be found in Appendix [12].)
Theorem 4. For any general loss function $D$ satisfying the conditions in Sec. 2 in the kernel regime, the gradient flow of both $h(x, t)$ and $h_{AS}(x, \Theta(t))$ follows the kernel dynamics

\[ \partial_t h' = -K(\cdot, X)\nabla h(x, t)D(h'(X, Y)), \]

with initial value $h'(0) = h_{ini} = h(x, t(0))$ and $h'(0) = 0$, respectively, where $\{X; Y\}$ is the training set, $K(x, x') = K_{0}(x, x') = \nabla \theta h(x, \theta_{0}) \cdot \nabla \theta h(x', \theta_{0})$.

Note that Chizat & Bach (2018) proposes a “doubling trick” to offset the initial DNN output, that is, neurons in the last layer are duplicated, with the new neurons having the same input weights but opposite output weights. By applying the “doubling trick”, $h'_{d}(0) = 0$. However, the kernel of layers $H - 1$ and $H$ doubles, whereas the kernel of layers $m \leq H - 2$ completely vanishes (See Appendix 13 for the proof), which could have large impact on the training dynamics as well as the generalization performance of DNNs.

7 Experiments

Our above theoretical results are obtained using the linearized model of DNN in Eq. (1) that well approximates the behavior of DNN in the kernel regime. In this section, we will demonstrate experimentally the accuracy of these results for very wide DNNs and the effectiveness of these results for general DNNs. First, using synthetic data, we verify the invariance of DNN output after experimentally the accuracy of these results for very wide DNNs and the effectiveness of these approximates the behavior of DNN in the kernel regime. In this section, we will demonstrate

7.1 Invariance of DNN output to loss functions

For a DNN $h(x, \theta(t))$ with initialization fixed at certain $\theta(0) = \theta_{0}$, we consider its gradient descent training for two loss functions: the $L^{2}$ (MSE) loss $D(h(X, \theta), Y) = \frac{1}{M} \sum_{i=1}^{M} (h(x_{i}, \theta) - y_{i})^{2}$ and the $L^{4}$ loss $D(h(X, \theta), Y) = \frac{1}{M} \sum_{i=1}^{M} (h(x_{i}, \theta) - y_{i})^{4}$. In Fig. 1, as Theorems 5 and 8 predict, the well-trained DNN outputs for these two losses overlap very well not only at 4 training points, but also at all the test points.

7.2 Linear relation and the effectiveness of ASI trick

7.2.1 1-d synthetic data

In this sub-section, we use 1-d data, which is convenient for visualization, to train DNNs of a large width. As shown in Fig. 2, without applying any trick, the original DNN initialized with a large weight learns/interpolates the training data in a fluctuating manner (blue solid). Both the ASI trick
We verify our theoretical results for high dimensional regression problems using Boston house price dataset (Harrison Jr & Rubinfeld 1978), in which we normalize the value of each property and the price to $[-0.5, 0.5]$. We choose 400 samples as the training data, and the other 106 samples as the test data. As illustrated by the red dots concentrating near the black line of an identity relation in Fig. 7.2.2, the RHS of Eq. (6) well predicts the final output of the original DNN without any trick, which is significant different from the final output of DNN with the ASI trick applied as shown by the blue dots deviating from the black line. As shown in 7.2.2, similar to the experiments on 1-d synthetic data, the ASI trick accelerates the training. In addition, conforming with Theorem 3, the generalization error of the DNN with ASI trick applied is much smaller than that of the original DNN.

7.2.2 Boston house price dataset

We verify our theoretical results for high dimensional regression problems using Boston house price dataset (Harrison Jr & Rubinfeld 1978), in which we normalize the value of each property and the price to $[-0.5, 0.5]$. We choose 400 samples as the training data, and the other 106 samples as the test data. As illustrated by the red dots concentrating near the black line of an identity relation in Fig. 7.2.2, the RHS of Eq. (6) well predicts the final output of the original DNN without any trick, which is significant different from the final output of DNN with the ASI trick applied as shown by the blue dots deviating from the black line. As shown in 7.2.2, similar to the experiments on 1-d synthetic data, the ASI trick accelerates the training. In addition, conforming with Theorem 3, the generalization error of the DNN with ASI trick applied is much smaller than that of the original DNN.
Figure 3: Boston house price dataset. (a) Each dot represents outputs evaluated at one test point. The abscissa is $h_K(\cdot; h_{\text{ini}}, X, Y)$ obtained using the original DNN. The ordinate for each blue dot is $h_K(x; 0, X, Y)$ obtained using DNN with the ASI trick applied, whereas for each red dot is the RHS of Eq. (6). The black line indicates the identity function $y = x$. (b) The evolution of training loss (blue solid) and test loss (red dashed) of the original DNN, and the training loss (black solid) and test loss (yellow dashed) of DNN with ASI trick applied. The width of DNN is 13-100000-1. $\sigma_{\text{std}} = 5$.

Figure 4: Effectiveness of ASI trick for MNIST dataset in the non-kernel regime of DNN. (a) Evolution of loss functions with the same legend as in Fig. 3(b). (b) Evolution of the corresponding accuracy. The learning rate is $2 \times 10^{-7}$. See main text for other settings.

7.2.3 MNIST dataset and the non-kernel regime of DNN

Next, we use the MNIST dataset to examine the effectiveness of ASI trick in the non-kernel regime of DNNs. We use a DNN with a more realistic setting of width 784-400-400-400-400-10, cross-entropy loss, batch size 512, and Adam optimizer (Kingma & Ba 2014). In such a case, as shown in Fig. 4, the ASI trick still effectively eliminate $h_{\text{ini}}$, accelerate the training speed and improve the generalization. In Fig. 4(b), with the ASI trick applied, both training and test accuracy exceeds 90% after only 1 epoch of training. This phenomenon further demonstrate that, without the interference of $h_{\text{ini}}$, DNNs can capture very efficiently and accurately the behavior of the training data.

8 Discussion

In this work, focusing on the regression problem, we propose a kernel-norm minimization framework to study theoretically the role of loss function and initialization for DNNs in the kernel regime. We prove that, given initialization, DNNs of different loss functions in a general class find the same global minimum. Regarding initialization, we find that a non-zero initial output of DNN leads to a specific type of generalization error. We then propose the ASI trick to eliminate this error without changing the neural tangent kernel. Experimentally, we find that ASI trick significantly accelerates the training and improves the generalization performance. Moreover, ASI trick remains effective for classification problems as well as for DNNs in the non-kernel regime. Because the error of DNN output induced by random initialization shrinks during the training, the advantage of ASI trick is much more significant at the early stage of the training. Based on above results, we suggest incorporating ASI trick in the design of controlled experiments for the quantitative study of DNNs.
From the perspective of training flexibility, ASI trick can alleviate the sensitivity of generalization and training speed to different random initializations of DNNs, thus expand the range of well-generalized initializations. This property could be especially helpful for finding a well-generalized solution of a new problem when empirical guidance is not available. We also remarks that, from Eq. (6), a particular prior of $h_{ini}$, such as the one from meta learning (Rabinowitz 2019), could decrease the generalization error. However, when meta learning is not available, a zero $h_{ini}$ is in general the best choice for generalization.

Cross-entropy loss is commonly used in classification problems, for which the DNN outputs are often transformed by a softmax function to stay in $(0,1)$. Theoretically, to obtain a zero cross-entropy loss given that labels of the training data take 1 or 0, weights of the DNN should approach infinity. In such a case, it is impossible for a DNN to stay in the kernel regime, which requires a small variation of weights throughout the training. However, in practice, training of a DNN often stops by meeting certain criteria of training accuracy or validation accuracy. Therefore, it is possible that weights of a sufficiently wide DNN stay in a small neighborhood of the initialization during the training. By setting a proper tolerance for the cross-entropy loss, we will analyze in the future the behavior of DNNs in kernel regime for classification problems with cross-entropy loss.
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Appendix

9 Notations

Ω: a compact domain of \( \mathbb{R}^{N_f} \); \( N_f \): dimension of input of DNN; \( f \): target function, \( f \in L^\infty(\Omega) \); \( N_p \): number of parameter of DNN; \( M \): number of training samples; \( X \): inputs of training set \( [x_1, \ldots, x_M]^T \in \mathbb{R}^{M \times N_f} \); \( Y \): outputs of training set \( [y_1, \ldots, y_M]^T \in \mathbb{R}^M \); \( g(x) \): \( g(x_1), \ldots, g(x_M) \)

for any function \( g \) on \( \Omega \); \( h_{\text{DNN}}(\cdot; \theta_{\text{DNN}}) \): output of DNN of parameters \( \theta_{\text{DNN}} \) at \( x \); \( \nabla_g(\cdot) \): \( \theta_{\text{DNN}}, \ldots, \theta_{\text{DNN}} \); \( h(x, \theta) \): linearized model of DNN defined by Eq. (9), \( D \): a general differentiable loss function satisfying conditions (i)--(iii) in Section 3.1; \( K \): inner product of space \( \mathcal{H}_K(\Omega) \); \( \| \cdot \|_K \): norm of space \( \mathcal{H}_K(\Omega) \); \( h_K(x; h, Y) \): the solution of problem (9) depending on kernel \( K \), initial function \( h \), inputs \( X \) and outputs \( Y \) of training set.

10 Theorems for the kernel-norm minimization framework

Theorem 5. Let \( \theta(t) \) be the solution of gradient flow dynamics

\[
\frac{d}{dt} \theta(t) = -\nabla \phi(h(X, \theta_0)^T \nabla h(X, \theta(t)) \cdot D(h(X, \theta(t)), Y)
\]

with initial value \( \theta(0) = \theta_0 \), where \( \nabla \phi(h(X, \theta_0)^T \nabla h(X, \theta(t)) \cdot D(h(X, \theta(t)), Y) \)

is a full rank \( ( \mathbb{R}^{N_p \times M} \) with \( N_p > M \). Then \( \theta(\infty) = \lim_{t \to \infty} \theta(t) \) exists and uniquely solves the constrained optimization problem

\[
\min_{\theta} \| \theta - \theta_0 \|_2, \text{ s.t., } h(X, \theta) = Y.
\]

Remark. Compared with the nonlinear gradient flow of DNN, the linearization in Eq. (9) is only performed on the hypothesis function \( h \) but not on the loss function or the gradient flow.

Proof. Gradient flow Eq. (9) can be written as

\[
\frac{d\theta(t)}{dt} = -\nabla \phi \cdot D(h(X, \theta(t)), Y).
\]

Then denote \( L(t) = D(h(X, \theta(t)), Y) \),

\[
\left| \frac{d\theta}{dt} \right|^2 = -\frac{d}{dt} L(t).
\]

Note that \( L(t) = D(h(X, \theta(t)), Y) \geq 0 \) for any \( t \geq 0 \). Then

\[
\int_0^\infty \left| \frac{d\theta}{dt} \right|^2 dt = L(0) - L(\infty) \leq L(0).
\]

Since \( \frac{d\theta}{dt} \) is continuous,

\[
\lim_{t \to \infty} \frac{d\theta(t)}{dt} = \lim_{t \to \infty} -\nabla \phi \cdot h(X, \theta_0)^T \nabla h(X, \theta(t)) \cdot D(h(X, \theta(t)), Y) = 0.
\]

Because \( \nabla \phi \cdot h(X, \theta_0)^T \) is a full rank matrix,

\[
\lim_{t \to \infty} \nabla h(X, \theta(t)) \cdot D(h(X, \theta(t)), Y) = 0.
\]

Recall that \( \nabla_z D(z', z) = 0 \) if and only if \( z' = z \),

\[
\lim_{t \to \infty} h(X, \theta(t)) = Y.
\]

By applying singular value decomposition to \( \nabla \phi \cdot h(X, \theta_0)^T \), we obtain \( \nabla \phi \cdot h(X, \theta_0)^T = V \Sigma U^T \), where \( V \) and \( U \) are orthonormal matrix of size \( N_p \times N_p \) and \( M \times M \) respectively, \( \Sigma = \begin{bmatrix} \Sigma_1 & \mathbf{0} \\
\mathbf{0} & \mathbf{0} \end{bmatrix} \) of size \( N_p \times M \).
where $\Sigma_1$ is a full rank diagonal matrix of size $M \times M$. $V$ can be split into two part as $V = [V_1, V_2]$, where $V_1$ takes the first $M$ columns and $V_2$ takes the last $N_p - M$ columns of $V$. Then

$$
\nabla_x h(X, \theta_0)^T = V \Sigma U^T = [V_1, V_2] \begin{bmatrix} \Sigma_1 \\ 0 \end{bmatrix} U^T
$$

$$
= V_1 \Sigma_1 U^T,
$$

$$
V_2^T \nabla_x h(X, \theta_0)^T = V_2^T V_1 \Sigma_1 U^T
$$

hence

$$
\frac{d}{dt} V_2^T \theta(t) = -V_2^T \nabla_x h(X, \theta_t) \nabla h(X, \theta_t) D(h(X, \theta_t), Y) = 0.
$$

which leads to

$$
V_2^T (\theta(t) - \theta_0) = 0, \text{ for any } t \geq 0.
$$

By Eq. (1), $\lim_{t \to \infty} h(X, \theta(t)) = Y$ yields

$$
\lim_{t \to \infty} \nabla_x h(X, \theta_t) (\theta(t) - \theta_0) = Y - h(X, \theta_0),
$$

which can be written as

$$
\lim_{t \to \infty} U \Sigma_1 V_1^T (\theta(t) - \theta_0) = Y - h(X, \theta_0)
$$

hence

$$
\lim_{t \to \infty} V_1^T (\theta(t) - \theta_0) = \Sigma_1^{-1} U^T [Y - h(X, \theta_0)].
$$

Combining Eq. (11) and (12), $\theta(\infty) = \lim_{t \to \infty} \theta(t)$ exists and is uniquely determined as

$$
V^T (\theta(\infty) - \theta_0) = \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix} (\theta(\infty) - \theta_0)
$$

$$
= \begin{bmatrix} \Sigma_1^{-1} U^T [Y - h(X, \theta_0)] \\ 0 \end{bmatrix},
$$

$$
\theta(\infty) - \theta_0 = V \begin{bmatrix} \Sigma_1^{-1} U^T [Y - h(X, \theta_0)] \\ 0 \end{bmatrix} = V_1 \Sigma_1^{-1} U^T [Y - h(X, \theta_0)],
$$

which leads to

$$
\theta(\infty) = V_1 \Sigma_1^{-1} U^T [Y - h(X, \theta_0)] + \theta_0.
$$

On the other hand, by the above analysis, problem (10) can be formulated as

$$
\min_{\theta} \|\theta - \theta_0\|_2, \text{ s.t. } V_1^T (\theta - \theta_0) = \Sigma_1^{-1} U^T [Y - h(X, \theta_0)].
$$

Any $\theta$ satisfies above constraint can be expressed as

$$
\theta = V_1 \Sigma_1^{-1} U^T [Y - h(X, \theta_0)] + V_2 \xi + \theta_0,
$$

where $\xi \in \mathbb{R}^{N_p - M}$. Then

$$
\|\theta - \theta_0\|_2^2 = \|V_1 \Sigma_1^{-1} U^T [Y - h(X, \theta_0)]\|_2^2 + \|V_2 \xi\|_2^2.
$$

Clearly, $\|\theta - \theta_0\|_2$ attains minimum if and only if $\xi = 0$. Therefore $\theta(\infty) = V_1 \Sigma_1^{-1} U^T [Y - h(X, \theta_0)] + \theta_0$ uniquely solves problem (10).

For the proof of Theorem 8 we first introduce the following two lemmas.

**Lemma 6.** For any $h' \in \mathcal{H}_K(\Omega)$, there exist $\theta' = (h'(\cdot), \nabla_x h(\cdot, \theta_0))^T_K$ such that $h' = \nabla_x h(x, \theta_0) \theta'$.

**Proof.** For any $h' \in \mathcal{H}_K(\Omega)$,

$$
\langle h'(\cdot), K(\cdot, \cdot) \rangle_K = \langle h'(\cdot), \nabla_x h(\cdot, \theta_0) \nabla_x h(z, \theta_0)^T \rangle_K
$$

$$
= \langle h'(\cdot), \nabla_x h(\cdot, \theta_0) \rangle_K \nabla_x h(z, \theta_0)^T
$$

For $\theta' = (h'(\cdot), \nabla_x h(\cdot, \theta_0))^T_K$, by the property of reproducing kernel $K$,

$$
h'(x) = \langle h'(\cdot), K(\cdot, x) \rangle_K = \nabla_x h(x, \theta_0) \theta'.
$$

$\Box$
Lemma 7. For any $\theta' \in \mathbb{R}^N$, $\nabla_{\theta} h(\cdot, \theta_0)\theta' \in \mathcal{H}_K(\Omega)$.

Proof. By the Mercer's theorem,
\[ K(x, y) = \sum_{j=1}^{\infty} \sigma_j \phi_j(x) \phi_j(y), \]
where $\{\phi_j\}_{j=1}^{\infty}$ are orthonormal basis of $L^2(\Omega)$. If $\nabla_{\theta} h(\cdot, \theta_0)\theta' \notin \mathcal{H}_K(\Omega)$, then there exist $j_1$ such that $\sigma_{j_1} = 0$ and $\langle \nabla_{\theta} h(\cdot, \theta_0)\theta', \phi_{j_1} \rangle_{L^2(\Omega)} \neq 0$. Then there exist $j_2$ such that $\langle \nabla_{\theta} h(\cdot, \theta_0)\phi_{j_1} \rangle_{L^2(\Omega)} \neq 0$, where $\theta_{j_2}$ is the $j_2$-th component of $\theta$. Then
\[
\int_{\Omega} \phi_{j_1}(x) K(x, x') \phi_{j_1}(x') dx' = \int_{\Omega} \phi_{j_1}(x) \left( \nabla_{\theta} h(\cdot, \theta_0)^T \nabla_{\theta} h(x', \theta_0) \right) \phi_{j_1}(x') dx'
= \sum_i \langle \partial_{\theta_i} h(\cdot, \theta_0), \phi_{j_1} \rangle_{L^2(\Omega)}^2 
\geq \langle \partial_{\theta_{j_2}} h(\cdot, \theta_0), \phi_{j_1} \rangle_{L^2(\Omega)}^2
> 0.
\]
However, on the other hand,
\[
\int_{\Omega} \phi_{j_1}(x) K(x, x') \phi_{j_1}(x') dx' = \int_{\Omega} \phi_{j_1}(x) \sum_{j=1}^{\infty} \sigma_j \phi_j(x) \phi_j(x') \phi_{j_1}(x') dx'
= \sum_j \langle \phi_j, \phi_{j_1} \rangle_{L^2(\Omega)}^2 
= \sigma_j
= 0,
\]
which leads to a contradiction. Therefore, $\nabla_{\theta} h(\cdot, \theta_0)\theta' \in \mathcal{H}_K(\Omega)$.

Theorem 8. Let $\theta$ be the solution of problem (10) then $h(x, \theta)$ uniquely solves the optimization problem
\[
\min_{h-h_{\text{ini}} \in \mathcal{H}_K(\Omega)} \|h - h_{\text{ini}}\|_K, \quad \text{s.t.} \quad h(X) = Y,
\]
where $h_{\text{ini}} = h(x, \theta_0)$ and the constraints $h(X) = Y$ are in the sense of trace $[Evans2010]$.

Proof. By Eq. (11) $h(x, \theta) - h_{\text{ini}} = \nabla_{\theta} h(x, \theta_0)(\theta - \theta_0)$. By Lemma 7 $h(\cdot, \theta) - h_{\text{ini}} \in \mathcal{H}_K(\Omega)$; for any $h - h_{\text{ini}} \in \mathcal{H}_K(\Omega)$, by lemma 6 for $\theta' = \langle h - h_{\text{ini}}, \nabla_{\theta} h(\cdot, \theta_0) \rangle_K^T$, $h - h_{\text{ini}} = \nabla_{\theta} h(x, \theta_0)\theta'$. Then
\[
\|h - h_{\text{ini}}\|_K = \|\nabla_{\theta} h(\cdot, \theta_0)\theta'\|_K
= \sqrt{\langle h - h_{\text{ini}}, \nabla_{\theta} h(\cdot, \theta_0)\theta' \rangle_K^T}
= \sqrt{\langle h - h_{\text{ini}}, \nabla_{\theta} h(\cdot, \theta_0) \theta' \rangle_K}
= \sqrt{\|\theta'\|^2_2}.
\]
By Problem 10, for any $\theta_1 \neq \theta - \theta_0$ that satisfies $h(X, \theta_1 + \theta_0) = Y$
\[
\|\theta_1\|_2 > \|\theta - \theta_0\|_2.
\]
Then, for problem (13), for any $h_1$ satisfying $h_1 - h_{\text{ini}} \in \mathcal{H}_K(\Omega)$, $h_1(X) = Y$ and $h_1(x) \neq h(x, \theta)$, let $\theta_1 = \langle h_1 - h_{\text{ini}}, \nabla_{\theta} h(\cdot, \theta_0) \rangle_K^T$. Clearly, $\theta_1 \neq \theta - \theta_0$, which leads to
\[
\|h_1 - h_{\text{ini}}\|_K = \|\theta_1\|_2 > \|\theta - \theta_0\|_2 = \|h(x, \theta) - h_{\text{ini}}\|_K.
\]
Therefore $h(x, \theta)$ uniquely solves problem (13). $\square$
Now, we obtain the equivalence between the long time solution of dynamics \(14\) and the solution of optimization problem \(15\) as follows.

**Corollary 9.** Let \(h(x,t)\) be the solution of dynamics

\[
\frac{d}{dt} h(x,t) = -K(x,X)\nabla h(X,t)D(h(X,t),Y),
\]

with \(h(x,0) = h(x,\theta_0)\) for certain \(\theta_0\). Then \(h(x,\infty)\) uniquely solves optimization problem

\[
\min_{h=h_{ini} \in \mathcal{H}_K(\Omega)} \|h-h_{ini}\|_K, \quad \text{s.t.,} \quad h(X) = Y.
\]

**Proof.** Notice that dynamics \(14\) is the same as dynamics \(3\) obtained from \(2\). Therefore, for \(h(x,0) = h(x,\theta_0), h(x,t) = h(x,\theta(t))\) where \(\theta(t)\) is the solution of dynamics \(2\) with initial condition \(\theta(0) = \theta_0\). By Theorem 5 and 8, \(h(x,\infty) = h(x,\theta(\infty))\) uniquely solves dynamics \(15\). \(\square\)

### 11 Impact of non-zero initial output

In this section, we use the above framework to show that a random non-zero initial DNN output leads to a specific type of generalization error. We begin with a lemma showing the linear composition property of the final DNN outputs in the kernel regime.

**Lemma 10.** For a fixed kernel function \(K : \Omega \times \Omega \rightarrow \mathbb{R}\), for any two training sets \(\{X;Y_1\}\) and \(\{X;Y_2\}\), where \(Y_1=[y_1^{(1)},\ldots,y_M^{(1)}]^T\) and \(Y_2=[y_1^{(2)},\ldots,y_M^{(2)}]^T\), the following linear relation holds

\[
h_K(\cdot;0,X,Y_1+Y_2) = h_K(\cdot;0,X,Y_1) + h_K(\cdot;0,X,Y_2).
\]

**Proof.** Let \(h_1(x,t), h_2(x,t)\) be the solutions of the gradient flow dynamics with respect to a MSE loss \(D(h(X,t),Y) = \frac{1}{2} \sum_{i=1}^M (h(x_i,t) - y_i)^2\)

\[
\frac{\partial}{\partial t} h(x,t) = -K(x,X)((h(x,t) - Y)
\]

with training labels \(Y = Y_1\) and \(Y = Y_2\), respectively, and \(h_1(x,0) = h_2(x,0) = h_{ini} = 0\). Then

\[
\begin{align*}
\partial_t (h_1 + h_2) &= -K(\cdot,X)(h_1(X,\theta(t)) - Y_1) - K(\cdot,X)(h_2(X,\theta(t)) - Y_2) \\
&= -K(\cdot,X)((h_1 + h_2)(X,\theta(t)) - (Y_1 + Y_2))
\end{align*}
\]

with initial value \((h_1 + h_2)(\cdot;0) = 0\). Therefore \(h_1 + h_2\) solves dynamics \(17\) for \(Y = Y_1 + Y_2\) and \(h_{ini} = 0\). Then, by Corollary 9 we obtain

\[
h_K(\cdot;0,X,Y_1+Y_2) = h_1(\cdot,\infty) + h_2(\cdot,\infty) = h_K(\cdot;0,X,Y_1) + h_K(\cdot;0,X,Y_2)
\]

\(\square\)

Using Lemma 10, we obtain the following quantitative relation between the solution with zero initial output and that with non-zero initial output.

**Theorem 11.** (Theorem 2 in main text) For a fixed kernel function \(K \in L^2(\Omega \times \Omega)\), and training set \(\{X;Y\}\), for any initial function \(h_{ini} \in L^\infty(\Omega)\), \(h_K(\cdot;h_{ini},X,Y)\) can be decomposed as

\[
h_K(\cdot;h_{ini},X,Y) = h_K(\cdot;0,X,Y) + h_{ini} - h_K(\cdot;0,X,h_{ini}(X)).
\]

**Proof.** Because \(h_K(\cdot;h_{ini},X,Y)\) is the solution of problem \(5\). Then \(h_K(\cdot;h_{ini},X,Y) - h_{ini}\) is the solution of problem

\[
\min_{h \in \mathcal{H}_K(\Omega)} \|h\|_K, \quad \text{s.t.,} \quad h(X) = Y - h_{ini}(X),
\]

whose solution is denoted as \(h_K(\cdot;0,X,Y-h_{ini}(X))\). By Lemma 10

\[
h_K(\cdot;0,X,Y-h_{ini}(X)) = h_K(\cdot;0,X,Y) - h_K(\cdot;0,X,h_{ini}(X)).
\]

Therefore

\[
h_K(\cdot;h_{ini},X,Y) = h_K(\cdot;0,X,Y-h_{ini}(X)) + h_{ini}
= h_K(\cdot;0,X,Y) + h_{ini} - h_K(\cdot;0,X,h_{ini}(X)).
\]

\(\square\)
The generalization error of DNN contributed by a random initial output can be estimated as follows.

**Theorem 12.** (Theorem 4 in main text) For a target function \( f \in L^\infty(\Omega) \), if \( h_{\text{ini}} \) is generated from an unbiased random function distribution \( P \) such that \( \mathbb{E}_{h_{\text{ini}} \sim P} h_{\text{ini}} = 0 \), then the generalization error of \( h_K(\cdot; h_{\text{ini}}, X, f(X)) \) can be decomposed as follows

\[
\mathbb{E}_{h_{\text{ini}} \sim P} L(h_K(\cdot; h_{\text{ini}}, X, f(X)), f) = L(h_K(\cdot; 0, X, f(X)), f) + \mathbb{E}_{h_{\text{ini}} \sim P} L(h_M(\cdot; 0, X, h_{\text{ini}}(X)), h_{\text{ini}}), \tag{21}
\]

where \( L(h_K(\cdot; h_{\text{ini}}, X, f(X)), f) = \|h_K(\cdot; h_{\text{ini}}, X, f(X)) - f\|_{L^2(\Omega)}^2 \| \cdot \|_{L^2(\Omega)} = \sqrt{\int_{\Omega} (\cdot)^2 \, dx} \).

**Proof.** By Theorem 11

\[
\|h_K(\cdot; h_{\text{ini}}, X, f(X)) - f\|_{L^2(\Omega)}^2 = \|h_K(\cdot; 0, X, f(X)) - f\|_{L^2(\Omega)}^2 + \|h_{\text{ini}} - h_K(\cdot; 0, X, h_{\text{ini}}(X))\|_{L^2(\Omega)}^2 + 2 \langle h_K(\cdot; 0, X, f(X)) - f, h_{\text{ini}} - h_K(\cdot; 0, X, h_{\text{ini}}(X))\rangle_{L^2(\Omega)}. \tag{22}
\]

Because \( \mathbb{E}_{h_{\text{ini}} \sim P} h_{\text{ini}} = 0 \), by Lemma 10, \( \mathbb{E}_{h_{\text{ini}} \sim P} \langle h_K(\cdot; 0, X, f(X)) - f, h_{\text{ini}} - h_K(\cdot; 0, X, h_{\text{ini}}(X))\rangle_{L^2(\Omega)} = 0 \),

\[
\mathbb{E}_{h_{\text{ini}} \sim P} L(h_K(\cdot; h_{\text{ini}}, X, f(X)), f) = L(h_K(\cdot; 0, X, f(X)), f) + \mathbb{E}_{h_{\text{ini}} \sim P} L(h_M(\cdot; 0, X, h_{\text{ini}}(X)), h_{\text{ini}}). \tag{24}
\]

\[ \square \]

### 12 AntiSymmetrical Initialization trick (ASI)

We design an AntiSymmetrical Initialization trick (ASI) which can make the initial output zero but also keep the kernel invariant. Let \( h_{i[l]} \) be the output of the \( l \)th node of the \( i \)th layer of a \( H \) layer DNN. Then, \( h_i^H(x) = \sigma^{[H]}_{i}([W_i^{[H]} \cdot h_i^{[H-1]}(x)]^2 + b_i^{[H]}) \), for \( i = 1, \ldots, n_l \). For the \( i \)th neuron of the output layer of DNN \( h_i^{[H]}(x) = W_i^{[H]} \cdot h_i^{[H-1]} + b_i^{[H]} \). After initializing the network with any conventional method, we obtain \( h^{[H]}(x, \theta(0)) \), where

\[
\theta(0) = [W^{[H]}(0), b^{[H]}(0), W^{[H-1]}(0), b^{[H-1]}(0), \ldots, b^{[1]}(0)].
\]

The ASI for general loss functions is to consider a new DNN with output \( h_{\text{ASI}}(x, \Theta(t)) = \sqrt{2} h^{[H]}(x, \theta(t)) - \sqrt{2} h^{[H]}(x, \theta'(t)) \) where \( \Theta = [\theta, \theta'] \), \( \Theta \) is initialized such that \( \theta'(0) = \theta(0) \). In following, we will prove that ASI trick eliminates the nonzero prior without changing the kernel \( K \).

**Theorem 13.** (Theorem 4 in main text) By applying trick ASI to any DNN \( h(x, \theta(t)) \) initialized by \( \theta(0) = \theta_0 \) such that \( h_{\text{ini}} = h(x, \theta_0) \neq 0 \), we obtain a new DNN \( h_{\text{ASI}}(x, \Theta(t)) = \sqrt{2} h(x, \theta_1(t)) - \sqrt{2} h(x, \theta_2(t)) \) (\( \Theta = [\theta_1, \theta_2] \)) with initial value \( \theta_1(0) = \theta_2(0) = \theta_0 \). Then, for any general loss function \( D \), in the kernel regime, the evolution of both \( h(x, \theta(t)) \) and \( h_{\text{ASI}}(x, \Theta(t)) \) under gradient flow of both DNNs follows kernel dynamics

\[
\partial_t h' = -K(\cdot, X)\nabla_{h(x,t)}D(h'(X,t), Y), \tag{25}
\]

with initial value \( h'(\cdot, 0) = h_{\text{ini}} \) and \( h' \neq 0 \), respectively, where \( \{X, Y\} \) is the training set, \( K(x, x') = K_{\theta_0}(x, x') = \nabla_\theta h(x, \theta_0) \cdot \nabla_\theta h(x', \theta_0) \).

**Proof.** Clearly, \( h(x, \theta(t)) \) under gradient flow follows dynamics (25) with initial function \( h'(\cdot, 0) = h_{\text{ini}} \). For the evolution of \( h_{\text{ASI}}(x, \Theta(t)) \), it is easy to see that it follows dynamics (25) with initial function...
\( h'(0) = 0 \) if and only if \( h_{\text{ASI}}(\cdot, \Theta(0)) = 0 \) and \( K_{\Theta_0} = K_{\Theta_0} \). By the definition of \( K_{\Theta_0} \),
\[
K_{\Theta_0}(x, x') = \nabla_{\Theta} h_{\text{ASI}}(x, \Theta(0)) \cdot \nabla_{\Theta} h_{\text{ASI}}(x', \Theta(0))
\]
\[
= \left[ \frac{\sqrt{2}}{2} \nabla_{\theta_1} h(x, \theta_1(0)) - \frac{\sqrt{2}}{2} \nabla_{\theta_2} h(x, \theta_2(0)) \right] \cdot \left[ \frac{\sqrt{2}}{2} \nabla_{\theta_1} h(x', \theta_1(0)) - \frac{\sqrt{2}}{2} \nabla_{\theta_2} h(x', \theta_2(0)) \right]
\]
\[
= \frac{1}{2} \nabla_{\theta_1} h(x, \theta_1(0)) \cdot \nabla_{\theta_1} h(x', \theta_1(0)) + \frac{1}{2} \nabla_{\theta_1} h(x, \theta_2(0)) \cdot \nabla_{\theta_1} h(x', \theta_2(0))
\]
\[
= \frac{1}{2} \nabla_{\theta_1} h(x, \theta_0) \cdot \nabla_{\theta_1} h(x', \theta_0) + \frac{1}{2} \nabla_{\theta_1} h(x, \theta_0) \cdot \nabla_{\theta_1} h(x', \theta_0)
\]
\[
= \nabla_{\theta_1} h(x, \theta_0) \cdot \nabla_{\theta_1} h(x', \theta_0) = K_{\Theta_0}.
\]

Moreover,
\[
h_{\text{ASI}}(x, \Theta(0)) = \frac{\sqrt{2}}{2} h(x, \theta_1(0)) - \frac{\sqrt{2}}{2} h(x, \theta_2(0)) = \frac{\sqrt{2}}{2} h(x, \theta_0) - \frac{\sqrt{2}}{2} h(x, \theta_0) = 0.
\]

Therefore, we prove the theorem. \( \square \)

13 “doubling trick”

By applying the “doubling trick” (Note that, in [Chizat & Bach, 2018], there is no bias term in the last layer), we obtain a new network with network parameters \( \theta' = \left[ W[H], W'[H-1], b'[H-1], \ldots, b'[1] \right] \) initialized as \( W[H](0) = [W[H](0); -W[H](0)], W'[H-1](0) = [W[H-1](0); W[H-1](0)], b'[H-1](0) = [b[H-1](0), b[H-1](0)] \) and \( W[l](0) = [0], b[l](0) = [0] \) for any \( l = 1, \ldots, H - 2 \).

In general, the kernel can be decomposed as the summation of kernels with respect the tangent space of parameters of the neural network in each layer, that is
\[
K_{\theta}(x, x') = \nabla_{\theta} h(x, \theta) \cdot \nabla_{\theta} h(x', \theta)
\]
\[
= \sum_{l=1}^{H} \left[ \nabla_{W[l]} h(x, \theta) \cdot \nabla_{W[l]} h(x, \theta) + \nabla_{b[l]} h(x, \theta) \cdot \nabla_{b[l]} h(x, \theta) \right].
\]

**Theorem 14.** For the DNN initialized by \( \theta' \), by applying the “doubling trick”, for any \( m \leq H - 2 \),
\[
K_{W[m]}(x, x') = 0, \quad K_{b'[m]}(x, x') = 0.
\]

For \( m = H - 1, H \), and \( \Theta = W[H-1], b[H-1], W[H] \),
\[
K_{\Theta'}(x, x') = 2K_{\Theta}(x, x'),
\]

**Proof.** For any \( m \leq H - 2 \),
\[
\nabla_{W[m]} h'(x, \theta'(0)) = \left( \prod_{i=m+1}^{H-1} W[i+1](0)s_i'[l](x, 0) W[j+1](0)s_j[l](x, 0) h_{j}[m-1](x, 0) \right)
\]
\[
\nabla_{b'[m]} h'(x, \theta'(0)) = \left( \prod_{i=m+1}^{H-1} W[i+1](0)s_i[l](x, 0) W[j+1](0)s_j[l](x, 0) \right)
\]
where \( s_i'[l](x, t) = s(W_i[l](t); h_{i}[l-1](x) + b_i[l](t)) \), for \( i = 1, \ldots, n_i \), \( s(x) = \frac{\partial r(x)}{\partial x} \). Because \( W[H](0)s[H-1](x, 0) = W[H](0)s[H-1](x, 0) - W[H](0)s[H-1](x, 0) = 0 \), for any \( m \leq H - 2 \), we obtain \( \nabla_{W[m]} h'(x, \theta'(0)) = 0 \) and \( \nabla_{b'[m]} h'(x, \theta'(0)) = 0 \), which leads to \( K_{W[m]}(x, x') = 0 \) and \( K_{b'[m]}(x, x') = 0 \). For layer \( H - 1 \) and \( H \), similarly, we have
\[
K_{W[H-1]}(x, x') = 2K_{W[H-1]}(x, x'),
\]
\[ K_{B^{[H-1]}H}(x, x') = 2K_{B^{[H-1]}H}(x, x'), \]
\[ K_{W^{[H]}H}(x, x') = 2K_{W^{[H]}H}(x, x'). \]

Therefore, by applying the “doubling trick”, \( h'(x, \theta(0)) \) is offset to 0. However, the kernel of layers \( H - 1 \) and \( H \) doubles, whereas the kernel of layers \( m \leq H - 2 \) completely vanishes, which could have large impact on the training dynamics as well as the generalization performance of DNN output.