A Dynamical View on Optimization Algorithms of Overparameterized Neural Networks

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Abstract

When equipped with efficient optimization algorithms, the over-parameterized neural networks have demonstrated high level of performance even though the loss function is non-convex and non-smooth. While many works have been focusing on understanding the loss dynamics by training neural networks with the gradient descent (GD), in this work, we consider a broad class of optimization algorithms that are commonly used in practice. For example, we show from a dynamical system perspective that the Heavy Ball (HB) method can converge to global minimum on mean squared error (MSE) at a linear rate (similar to GD); however, the Nesterov accelerated gradient descent (NAG) only converges to global minimum sublinearly.

Our results rely on the connection between neural tangent kernel (NTK) and finite over-parameterized neural networks with ReLU activation, which leads to analyzing the limiting ordinary differential equations (ODE) for optimization algorithms. We show that, optimizing the non-convex loss over the weights corresponds to optimizing some strongly convex loss over the prediction error. As a consequence, we can leverage the classical convex optimization theory to understand the convergence behavior of neural networks. We believe our approach can also be extended to other loss functions and network architectures.

1 Introduction

Neural Tangent Kernel (NTK) [34] has taken a huge step in understanding the behaviors of over-parameterized (or wide) and deep neural networks: it has been shown that the training process of a neural network can be characterized by a kernel matrix. Although the NTK matrix is randomly initialized and time-dependent, it in fact stays close to a constant limiting kernel matrix, on which the analysis of neural networks renders much easier. Leveraging NTK, researches have extensively studied how different aspects affect the convergence of training neural networks. For example, weight initialization with large variance can accelerate the convergence but worsen the generalization ability of neural networks [21, 62]. It has been analyzed in [22] that a two-layer fully-connected neural networks (FCNN) with ReLU

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activation provably and globally converges to zero training loss. Later the results are enriched by extending the global convergence to multi-layer (deep) FCNN, convolutional neural networks (CNN), recurrent neural networks (RNN) and residual neural networks (ResNet) \[22, 3, 7, 4\]. Especially, the comprehensive result in \[3\] covers all above-mentioned network architectures, as well as different losses such as mean square error (MSE) and cross-entropy. Specifically, the over-parameterized neural networks enjoy an exponentially decaying MSE and a polynomially decaying cross-entropy. Other examples studied the convergence with NTK under different input distribution \[22, 3, 20\], activation functions \[20\] and normalization layers \[24\].

There are also a wealth of recent literature on the generalization properties of the wide neural networks based on NTK. For example, using a data-dependent Rademacher complexity measure, a generalization bound independent of network size for a two-layer, ReLU activated, FCNN can be obtained \[45, 6, 2\]. Several lines of work \[11, 44, 19\] gave spectrally-normalized margin-based generalization bound to explain the nice generalization phenomenon of over-parameterized networks. The others \[25, 44, 41\] derived the generalization bound from the view of PAC-Bayes and compression approaches. More examples include the generalization bound for high dimension data \[1, 28\] and with weight decay \[38\].

While many works have been focused on the convergence theory of neural network architectures, one would argue that the efficient optimization of a neural network is as important as the design of neural networks. Nevertheless, to our knowledge, this is the first paper to go beyond GD (and SGD) and analyze the global convergence of neural networks from a more general optimization algorithm perspective. In this work, we employ some state-of-the-art optimizers and analyze their convergence behavior under the NTK regime. A related work is \[39\], where authors also study GD with momentum under the NTK regime but only empirically. We seek to answer the following questions:

- Can different optimization algorithms beside GD provably find global minimum in the non-convex optimization of neural networks?
- Can we leverage classic convex optimization theory to explain the behavior (e.g. acceleration and rate) of optimization algorithms when training the neural networks?

Intriguingly, the known results of global and linear convergence of GD (and SGD) on MSE is somewhat surprising, since losses are non-convex with respect to weights. Note that the traditional convex optimization theory only claims \(O(1/t)\) rate of GD, even for convex losses, and we only achieve the linear convergence rate when the loss is strongly convex. This phenomenon suggests a close relationship between the non-convex optimization in neural networks and some convex optimization problems that we will elaborate in this paper. We establish such connection rigorously which allows us to conveniently employ the classic convex optimization theory at low cost, thus bridging both worlds to inspire new insights into the training of neural networks.

Once we view the evolution of neural networks during training as an ordinary differential equation (ODE), a.k.a. the gradient flow, there are plenty of fruitful results in the long history of convex optimization \[50, 13, 46, 53, 14, 56\]. We can consider different optimization algorithms, e.g. the Heavy Ball method (HB) \[51\], the Nesterov accelerated gradient descent (NAG) \[43\], subgradient descent, Newton’s method, GD with multiple momentums \[48\] and so on. Each optimization algorithm has a corresponding limiting ODE (see HB ODE \[51\] and NAG ODE \[59\]), which is equivalent to the discrete optimization algorithm with an infinitely
small step size. To analyze such ODEs, we can apply the Gronwall’s inequality \[30, 12\] for GD and the Lyapunov function or energy \[36, 61, 49\] for higher order ODE (which is incurred by employing the momentum terms \[52, 54\]).

Our contribution is two-fold: we show that the non-convex weight dynamics has the same form as a strongly-convex error dynamics, where Lyapunov functions are applicable; we prove that HB also enjoys global linear convergence with a rate faster than GD, and NAG converges at sublinear rate and requires more width than HB.

2 Preliminaries

In this section, we introduce the NTK approach to analyze the convergence behavior of any neural networks from a dynamical system perspective. Particularly, we warm ourselves up with some known results of training a two-layer neural network \[22\], using the MSE loss and the GD.

To start with, we do not specify the neural network architecture (e.g. layers, activation, depth, width, etc.). Given a training set \(\{x_i, y_i\}_{i=1}^n\) where \(x_i \in \mathbb{R}^p\), we denote the weights \(w_r \in \mathbb{R}^p\) as the weight vectors in the first hidden layer connecting to the \(r\)-th neuron, \(W\) as the union \(\{w_r\}\) and \(a\) as the set of weights in all the other layers. We write \(f(W, a, x_i)\) as the neural network output. We aim to minimize the MSE loss:

\[
L(W, a) = \frac{1}{2} \sum_{i=1}^{n} (f(W, a, x_i) - y_i)^2
\]

Taking the same route as in \[22\], we focus on optimizing \(W\) with \(a\) fixed at initialization\[1\]. Applying the simplest gradient descent with a step size \(\eta\), we have:

\[
w_r(k + 1) = w_r(k) - \eta \frac{\partial L(W(k), a)}{\partial w_r(k)}
\]

Since GD is a discretization of its corresponding ordinary differential equation (ODE, known as the gradient flow), we analyze such ODE directly as an equivalent form of GD with an infinitesimal step size. The gradient flows are dynamical systems that are much amenable to analyze and understand different optimization algorithms. To be specific, GD has a gradient flow as

\[
\frac{d w_r(t)}{dt} = - \frac{\partial L(W(t), a)}{\partial w_r(t)}
\]  

(2.1)

**Remark 2.1.** Different optimization algorithms may have the same limiting ODE: it has been shown in \[31\] that the forward Euler discretization of (2.1) gives GD, while the backward Euler discretization gives the proximal point algorithm \[47\]. Another example relating Nesterov accelerated gradient and Heavy Ball can be found in Section 3.

\[1\]In section 5.3 we extend our analysis to training all layers simultaneously. We remark that training only the first layer is sufficient to find the global minimum of loss.
Simple chain rule gives the following dynamics,
\[
\frac{dw_r(t)}{dt} = -\frac{\partial L}{\partial f(t)} \frac{\partial f(t)}{\partial w_r(t)} = -(f - y) \frac{\partial f(t)}{\partial w_r(t)}
\] (2.2)
\[
\frac{df(t)}{dt} = \sum_r \frac{\partial f(t)}{\partial w_r(t)} \frac{dw_r(t)}{dt} = -H(t)(f - y)
\] (2.3)
\[
\dot{\Delta}(t) = -H(t)\Delta(t)
\] (2.4)
which we refer to as the weight dynamics, the prediction dynamics and the error dynamics, respectively. Here we denote the error of the prediction \(\Delta = f - y \in \mathbb{R}^n\) and the \(\mathbb{R}^{n \times n}\) NTK matrix as \(H(t) := \sum_r \frac{\partial f(t)}{\partial w_r(t)} \left( \frac{\partial f(t)}{\partial w_r(t)} \right)^\top\) (2.5)
which is the sum of outer products.

The key observation of training the over-parameterized neural networks is that \(W(t)\) stays very close to its initialization \(W(0)\), even though the loss may change largely. This phenomenon is well-known as ‘lazy training’ [17, 34]. As a consequence, the neural network \(f\) is almost linear in \(W\) and the kernel \(H(t)\) behaves almost time-independently: \(\lim_{m \to \infty} H(0) \approx H(0) \approx H(t)\) [22, Remark 3.1].

Interestingly, suppose we define a pseudo-loss \(\hat{L}(t) := \frac{1}{2} \Delta^\top H \Delta\) and notice that \(L = \frac{1}{2} \Delta^\top \Delta\), then optimizing the non-convex loss \(L\) over \(w\) leads to an error dynamics \([2.4]\), as if we were actually optimizing a strongly-convex loss \(\hat{L}\) over \(\Delta\) with the same dynamical system as \([2.1]\):
\[
\frac{d\Delta(t)}{dt} = -\frac{\partial \hat{L}(W(t), a)}{\partial \Delta(t)}.
\]
The matrix ODE \([2.4]\) with a constant and positive \(H\) has a solution converging to 0 at linear rate, as the classical theory on optimizing a strongly convex loss indicates. In other words, optimizing the non-convex \(L\) for over-parameterized neural networks converges faster than optimizing convex losses and reaches the convergence speed of optimizing strongly convex losses. Therefore it is essential to show that \(H\) is positive with the smallest eigenvalue bounded away from 0 at all time. We formalize this claim by quoting the results for the two-layer neural network of the following form,
\[
f(W, a, x) = \frac{1}{\sqrt{m}} \sum_{r=1}^m a_r \sigma \left( w_r^\top x \right)
\]
with \(\sigma(z) = \max z, 0\) being the ReLU activation function. Now we quote an important fact that justifies our main theorem.

**Fact 2.2** (Assumption 3.1 and Theorem 3.1 in [22]). Define matrix \(H^\infty \in \mathbb{R}^{n \times n}\) with
\[
(H^\infty)_{ij} = \mathbb{E}_{w_r \sim N(0, I)} \left[ x_i^\top x_j \mathbb{I} \left\{ w_r^\top x_i \geq 0, w_r^\top x_j \geq 0 \right\} \right] = \left( \frac{1}{2} - \frac{\arccos(x_i^\top x_j)}{2\pi} \right) (x_i^\top x_j)
\]
and define \(\lambda_0 := \lambda_{\min}(H^\infty)\) as the smallest eigenvalue of \(H^\infty\). Suppose for any \(i \neq j\), \(x_i \parallel x_j\), then \(\lambda_0 > 0\).
Here $H^\infty$ is the limiting form at the initialization, i.e., $H^\infty = \lim_{m \to \infty} H(0)$. We note that the explicit formula $(H^\infty)_{ij} = \left(\frac{1}{2} - \frac{\arccos(x_i^\top x_j)}{2\pi}\right) (x_i^\top x_j)$ is given by [18] and especially $(H^\infty)_{ij} = 1/2$. In [22], the authors establish that, for sufficiently wide hidden layer and under some data distributional assumptions, GD converges to zero training loss exponentially fast. Formally, Theorem 1 (Theorem 3.2 and Lemma 3.2 in [22]). Suppose $\forall i, \|x_i\|_2 = 1$ and $|y_i| < C$ for some constant $C$, and only the hidden layer weights $\{w_r\}$ are optimized. If we set the width $m = \Omega(n^6/\lambda_0^4\delta^3)$ and we i.i.d. initialize $w_r \sim \mathcal{N}(0, I), a_r \sim \text{unif}\{-1, 1\}$ for $r \in [m]$, then with high probability at least $1 - \delta$ over the initialization, we have

$$\lambda_{\min}(H(t)) > \frac{1}{2} \lambda_{\min}(\lim_m H(0)) := \frac{1}{2} \lambda_{\min}(H^\infty) = \frac{\lambda_0}{2}$$

with $H^\infty$ defined in Fact 2.2 and the linear convergence

$$L(t) \leq \exp(-\lambda_0 t) L(0).$$

We note that the NTK matrix (2.5) is the Gram matrix induced by the ReLU activation:

$$H_{ij}(t) = \sum_{r=1}^m \frac{\partial f_i(t)}{\partial w_r} \left(\frac{\partial f_j(t)}{\partial w_r}\right)^\top = \frac{1}{m} x_i^\top x_j \sum_{r=1}^m I(w_r^\top x_i \geq 0, w_r^\top x_j \geq 0)$$

(2.6)

We remark that the framework of Theorem 1 has been extended to training multiple layers simultaneously [22] (see also Section 5.3). The analysis has recently been generalized to different network architectures and losses and we now complement this line of research by extending to different optimization algorithms. To present the simplest proof, we only analyze the continuous gradient flows and we believe our approach can be easily extended to the discrete time analysis.

3 Heavy Ball with Friction System

Our first result concerns the GD with momentum, or the Heavy Ball (HB) method [51]:

$$w_r(k+1) = w_r(k) - \eta \frac{\partial L(W(k), a_r)}{\partial w_r(k)} + \beta (w_r(k) - w_r(k-1))$$

(3.1)
or equivalently

$$w_r(k+1) = w_r(k) + \eta v(k)$$

$$v(k) = - \frac{\partial L(W(k), a_r)}{\partial w_r(k)} + \beta v(k-1)$$

(3.2)

where $\eta$ is the step size and the momentum term $\beta \in [0, 1]$. The corresponding gradient flow is known as the Heavy Ball with Friction (HBF) system. This is a non-linear dissipative dynamical system, originally proposed by [51] and heavily studied in [9, 26, 15, 8, 5, 61]: with $b > 0$

$$\dot{w}_r(t) + bw_r(t) + \frac{\partial L(W(t), a_r)}{\partial w_r(t)} = 0.$$
As shown later in Section 3.1, the error dynamics is
\[ \ddot{\Delta}(t) + b\dot{\Delta}(t) + \frac{\partial \hat{L}}{\partial \Delta(t)} = 0. \] (3.4)

We note that other optimization algorithms may also correspond to the HBF system: for example NAG-SC\(^2\) (Nesterov accelerated gradient descent for strongly convex objective in \(^61\)), though they are distinguishable using high resolution ODE \(^55\).

In particular, we study the case as in \(^61\), Equation (7) and \(^57\), when \[ b = \sqrt{2\lambda_0}, \] i.e. twice the strongly convexity of \( H(t) \):
\[ \dddot{w}_r(t) + \sqrt{2\lambda_0} \dot{w}_r(t) + \frac{\partial f}{\partial w_r}(f - y) = 0 \] (3.5)

Our choice of parameter \( b \) leads to a global linear convergence to zero training loss, without requiring Lipschitz gradients of \( \hat{L} \). For other choices of parameters with the Lipschitz condition of \( \hat{L} \), HB can enjoy linear converge locally \(^51\), \(^40\) and globally \(^43\), \(^27\), \(^60\), \(^57\), \(^10\).

To solve a second order ODE requires initial conditions on \( w_r \) and \( \dot{w}_r \), which we assume as \( \dot{w}_r(0) = 0 \) without loss of generality. Now we state the our main theorem under MSE loss.

**Theorem 2.** Suppose we set the width of the hidden layer \( m = \Omega \left( \frac{n^6}{\delta^3 \lambda_0^4} \right) \) and \( b = \sqrt{2\lambda_0} \). If we i.i.d. initialize \( w_r \sim \mathcal{N}(0, I) \), \( a_r \sim \text{unif}\{-1, 1\} \) for \( r \in [m] \), then with high probability at least \( 1 - \delta \) over the initialization, we have
\[ L(t) \leq \frac{4}{\lambda_0} \exp \left( -\sqrt{\lambda_0/2} \cdot t \right) \hat{L}(0). \]

We notice that indeed \( \sqrt{\lambda_0/2} > \lambda_0 \), suggesting a boost in the linear convergence rate of HB when compared to GD, as we observe in Figure 1. To prove this, we claim that \( \lambda_0 < 1/2 \) as \( \text{tr}(H^\infty) = n \cdot (H^\infty)_{ii} = n/2 = \sum \lambda_i > n\lambda_0 \), with \( \lambda_i \) representing the eigenvalues of \( H^\infty \). Another observation is that, to guarantee the linear convergence, HB requires the same order of width as GD in Theorem 1.

In the following section, we prove our theorem by employing the Lyapunov function.

### 3.1 Proof of Theorem 2

First, we use the chain rule to characterize the prediction dynamics of \( f \),
\[
\begin{align*}
\dot{f}_i(t) &= \sum_{r \in [m]} \frac{\partial f_i}{\partial w_r} \dot{w}_r, \\
\ddot{f}_i(t) &= \sum_{r, l \in [m]} \frac{\partial^2 f_i}{\partial w_r \partial w_l} \ddot{w}_l + \sum_{r \in [m]} \frac{\partial f_i}{\partial w_r} \dot{w}_r \overset{\text{a.s.}}{=} \sum_{r \in [m]} \frac{\partial f_i}{\partial w_r} \dot{w}_r.
\end{align*}
\]

\(^2\)Assuming \( \hat{L} \) is \( \mu \)-strongly convex, then the limiting ODE \( \ddot{\Delta}(t) + 2\sqrt{\mu} \dot{\Delta}(t) + \frac{\partial \hat{L}}{\partial \Delta(t)} = 0 \) corresponds to NAG-SC:
\[
\begin{align*}
v(k + 1) &= \Delta(k) - \eta \frac{\partial \hat{L}}{\partial \Delta(k)} \\
\Delta(k + 1) &= v(k + 1) + \frac{1 - \sqrt{\mu\eta}}{1 + \sqrt{\mu\eta}} (v(k + 1) - v(k)).
\end{align*}
\]
Figure 1: Logarithm MSE vs. epoch of HB on MNIST. We observe that HB shows faster linear convergence than GD. Details of experiments are left in Appendix D.1.

where the last equality follows from a key observation that, with $\delta(\cdot)$ denoting the Dirac Delta function,

$$
\frac{\partial f_i}{\partial w_r} = \frac{1}{\sqrt{m}} a_r x_i \| w_r^T x_i > 0),
$$

$$
\frac{\partial^2 f_i}{\partial w_r \partial w_l} = 0, \text{ for } l \neq r
$$

$$
\frac{\partial^2 f_i}{\partial w_r^2} = \frac{1}{\sqrt{m}} a_r x_i^T x_i \delta(w_r^T x_i) \overset{a.s.}{=} 0.
$$

Multiplying $\frac{\partial f_r}{\partial w_r}$ to (3.5) and sum over $r$, we obtain the prediction dynamics as

$$
\dot{f}(t) + \sqrt{2\lambda_0} \ddot{f}(t) + H(t)(f - y) = 0
$$

and consequently, the dynamics of the error is

$$
\dot{\Delta}(t) + \sqrt{2\lambda_0} \Delta(t) + H(t)\Delta(t) = 0 \quad (3.7)
$$

or in an analogous form to (3.5),

$$
\dot{\Delta}(t) + \sqrt{2\lambda_0} \Delta(t) + \frac{\partial \hat{L}}{\partial \Delta(t)} = 0
$$

To establish the linear convergence in MSE, we need to guarantee $H(t)$ is positive definite with $\lambda_{\min}(H(t)) \geq \lambda_0/2$ for all $t$. In other words, the pseudo loss $\hat{L}$ is $\frac{\lambda_0}{2}$-strongly convex. We start with $t = 0$, by showing that for wide enough neural networks, $H(0)$ has a positive smallest eigenvalue with high probability.

**Lemma 3.1** (Lemma 3.1 in [22]). If $m = \Omega \left( \frac{n^2}{\lambda_0^2} \log \left( \frac{n^2}{\delta} \right) \right)$, then we have $\|H(0) - H^{\infty}\|_2 \leq \frac{\lambda_0}{4}$ and $\lambda_{\min}(H(0)) \geq \frac{3}{4} \lambda_0$ with probability of at least $1 - \delta$. 7
Next, we introduce a lemma that shows for any \( t \), if \( w_r(t) \) is close to \( w_r(0) \), then \( H(t) \) is close to \( H(0) \). Together with Lemma 3.1, \( \lambda_{\min}(H(t)) \) always has a positive smallest eigenvalue. In words, the lazy training leads to the positive definiteness.

**Lemma 3.2** (Lemma 3.2 in [22]). If \( w_r \) are i.i.d. generated from \( \mathcal{N}(0, I) \) for \( r \in [m] \), and \( \|w_r(0) - w_r\|_2 \leq \frac{\delta}{m} =: R \) for some small positive constant \( c \), then the following holds with probability at least \( 1 - \delta \) we have \( \|H(t) - H(0)\|_2 < \frac{\lambda_0}{4} \) and \( \lambda_{\min}(H(t)) > \frac{\lambda_0}{2} \).

The next lemma gives two important facts given that \( \lambda_{\min}(H(s)) \) for previous time \( s \leq t \); the loss decays exponentially and weights stay close to their initialization at the current time \( t \). In other words, the positive definiteness indicates the convergence of the loss, which further indicates the lazy training. We emphasize that our Lemma 3.3 is specific to the choice of optimization algorithms and hence the proof is much different than its analog in [22, Lemma 3.3] for GD.

**Lemma 3.3.** Assume \( 0 \leq s \leq t \) and \( \lambda_{\min}(H(s)) \geq \frac{\lambda_0}{2} \). Then \( L(t) \leq \frac{4}{\lambda_0} \exp \left(-\sqrt{\lambda_0/2}t\right) L(0) \) and \( \|w_r(t) - w_r(0)\|_2 \leq \sqrt{\frac{32n L(0)}{9m \lambda_0^2}} =: R' \).

**Proof.** Borrowing the idea of [61, 57], we define the Lyapunov function or Lyapunov energy as

\[
V(t) := \hat{L} + \frac{1}{2} \left\| \sqrt{\frac{\lambda_0}{2}} \Delta(t) + \hat{\Delta}(t) \right\|^2 = \frac{1}{2} \Delta(t) \top H(t) \Delta(t) + \frac{1}{2} \left\| \sqrt{\frac{\lambda_0}{2}} \Delta(t) + \hat{\Delta}(t) \right\|^2.
\]

The Lyapunov function represents the total energy of the system and always decreases along the trajectory of the training dynamics since, as we will later show, \( \dot{V}(t) < 0 \). Here we simplify the notation by denoting the dependence on \( t \) in the subscript and use \( \alpha := b/2 = \sqrt{\lambda_0/2} \).

We derive by the chain rule,

\[
\dot{V}(t) = \dot{\Delta} \top H(t) \Delta(t) + \frac{1}{2} \Delta \top \dot{H}(t) \Delta(t) + \left\langle \alpha \dot{\Delta} + \hat{\Delta}, \alpha \Delta(t) + \hat{\Delta} \right\rangle,
\]

where we use \( \left\langle u, v \right\rangle = u \top v \) to denote the inner product.

Notice that by (2.6), we have \( \dot{H}(t) \approx 0 \). Substituting the error dynamics (3.7) for \( \dot{\Delta} \), we have

\[
\dot{V}(t) = \left\langle H \Delta(t), \dot{\Delta} \right\rangle + \left\langle -\alpha \dot{\Delta} - H \Delta(t), \alpha \Delta(t) + \hat{\Delta} \right\rangle = -\alpha \left\langle H \Delta(t), \Delta(t) \right\rangle - \alpha^2 \left\langle \Delta(t), \Delta(t) \right\rangle - \alpha \left\langle \Delta(t), \Delta(t) \right\rangle
\]

Using \( \lambda_{\min}(H) \geq \frac{\lambda_0}{2} = \alpha^2 \), we get

\[
\left\langle H \Delta(t), \Delta(t) \right\rangle \geq \frac{1}{2} \left\langle H \Delta(t), \Delta(t) \right\rangle + \frac{\alpha^2}{2} \left\langle \Delta(t), \Delta(t) \right\rangle = \hat{L}(t) + \frac{\alpha^2}{2} \left\langle \Delta(t), \Delta(t) \right\rangle
\]

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and hence we have
\[
\dot{V}(t) = -\alpha \dot{\hat{L}}(t) - \alpha^3 2 \langle \Delta_t, \Delta_t \rangle - \alpha^2 \langle \dot{\Delta}_t, \Delta_t \rangle - \alpha \langle \dot{\Delta}_t, \dot{\Delta}_t \rangle
\]
\[
< - \alpha \left( \hat{L}(t) + \frac{1}{2} \| \alpha \Delta_t + \dot{\Delta}_t \|^2 \right) = -\alpha V(t)
\]
where in the last inequality we throw away \(-\alpha^2 \langle \dot{\Delta}_t, \dot{\Delta}_t \rangle \). Clearly \(\dot{V}(t) \leq 0\) for all \(t\) since \(V(t)\) is by definition positive. For this first order scalar ODE, we apply the Gronwall’s inequality to derive that
\[
V(t) < e^{-\alpha t} V(0)
\]
and we obtain
\[
\hat{L}(t) \leq V(t) < e^{-\alpha t} V(0) = e^{-\alpha t} \left( \frac{1}{2} \Delta(0)^\top \Delta(0) + \frac{\alpha^2}{2} \| \Delta(0) \|^2 \right).
\]
Again using \(\lambda_{\text{min}}(H(0)) \geq \alpha^2\), we have
\[
\hat{L}(t) \leq \exp (-\alpha t) \left( \frac{1}{2} \Delta(0)^\top \Delta(0) + \hat{L}(0) \right) = 2 \exp (-\alpha t) \hat{L}(0)
\]
and
\[
L(t) \leq \frac{2}{\alpha^2} \exp (-\alpha t) \hat{L}(0).
\]
In words, the prediction \(f(t) \to y\) exponentially fast, with a convergence factor \(\alpha = \sqrt{\lambda_0}/2\).

Now we move on to show that \(w_r(t)\) stays close to \(w_r(0)\). Multiplying \(e^{bt} = e^{2\alpha t}\) to the weight dynamics (3.5), we have
\[
\frac{d}{dt} \left( e^{2\alpha t} \dot{w}_r \right) = -\frac{1}{\sqrt{m}} e^{2\alpha t} a_r \sum_i (f_i - y_i) x_i \mathbb{I}(w_r^\top x_i \geq 0)
\]
which gives a close-form solution
\[
\dot{w}_r = -e^{-2\alpha t} \int_0^t \frac{1}{\sqrt{m}} e^{2\alpha s} a_r \sum_i (f_i - y_i) x_i \mathbb{I}(w_r^\top x_i \geq 0) ds
\]
whose norm satisfies
\[
\| \dot{w}_r \| \leq e^{-2\alpha t} \frac{1}{\sqrt{m}} \int_0^t e^{2\alpha s} \sum_i |f_i(s) - y_i| ds
\]
\[
\leq e^{-2\alpha t} \sqrt{\frac{n}{m}} \int_0^t e^{2\alpha s} \| f(s) - y \|_2 ds
\]
\[
= \sqrt{\frac{n}{m}} \int_0^t e^{2\alpha (s-t)} \sqrt{L(s)} ds
\]
\[
\leq \sqrt{\frac{2n \hat{L}(0)}{m \alpha^2}} \int_0^t e^{2\alpha s - 2\alpha t} ds
\]
\[
\leq \sqrt{\frac{8n \hat{L}(0)}{9m \alpha^2}} e^{-\alpha t/2}
\]
Finally by Cauchy Schwarz, we bound the weight distance from initialization,
\[ \| w_r(t) - w_r(0) \|_2 \leq \int_0^t \| \dot{w}_r(s) \|_2 \, ds < \sqrt{\frac{32n\hat{L}(0)}{9m\alpha^6}}. \]

We quote the next lemma to show that \( R'(t) < R \) indicates that for all \( t > 0 \), the conditions in Lemma 3.2 and 3.3 hold. This lemma is closely related to [22, Lemma 3.4] and the proof is given in Appendix C.

**Lemma 3.4.** If \( R' < R \), then we have \( \lambda_{\min}(H(t)) \geq \frac{1}{2} \lambda_0 \), for all \( r \in [m] \), \( \| w_r(t) - w_r(0) \|_2 \leq R' \) and \( L(t) \leq \frac{1}{\lambda_0} \exp\left(-\frac{\sqrt{\lambda_0}}{2t}\right) \hat{L}(0) \).

Finally we study the width requirement for \( R' < R \) to hold true, i.e. we need \( \sqrt{\frac{32n\hat{L}(0)}{9m\alpha^6}} < O(\frac{\delta n^4}{\lambda_0}) \) which is equivalent to \( m = \Omega(\frac{n^6}{\delta^3 \lambda_0^4}) \). This is shown in Appendix A.2.

### 4 Nesterov Accelerated Gradient Descent

In this section, we analyze the dynamics of the generalized Nesterov Accelerated Gradient (NAG) descent as follows,

\[ v(k+1) = w_r(k) - \eta \frac{\partial L(W(k), a)}{\partial w_r(k)} \]  
\[ w_r(k+1) = v(k+1) + \frac{k-1}{k+d-1}(v(k+1) - v(k)) \]

where \( \eta \) is step size. It has been given in [59] that the corresponding gradient flow as

\[ \ddot{f}(t) + \frac{d}{dt} \dot{f}(t) + H(t)(f - y) = 0 \]  
\[ \ddot{\Delta}(t) + \frac{d}{dt} \dot{\Delta}(t) + H(t)\Delta(t) = 0 \]

With initial conditions \( \dot{w}_r(0) = 0 \), we multiply \( \frac{\partial f}{\partial w_r} \) to (4.2) and sum over \( r \). It follows from (3.6) that the prediction dynamics and the error dynamics are

\[ \ddot{f}(t) + \frac{d}{dt} \dot{f}(t) + H(t)(f - y) = 0 \]  
\[ \ddot{\Delta}(t) + \frac{d}{dt} \dot{\Delta}(t) + H(t)\Delta(t) = 0 \]

with the same NTK matrix \( H(t) \) as defined in (2.6). Again, using the pseudo-loss \( \hat{L}(t) \), we have an error dynamics that is analogous to the weight dynamics (4.2),

\[ \ddot{\Delta}(t) + \frac{d}{dt} \dot{\Delta}(t) + \frac{\partial \hat{L}}{\partial \Delta(t)} = 0. \]

We now state our convergence analysis of NAG based on this error dynamics.
Theorem 3. Suppose we set the width of the hidden layer $m = \Omega \left( \frac{n^{\alpha/2 - 4}}{\delta^{3\alpha/2 - 4} \lambda_{0}^{\alpha/2 - 2}} \right)$ where $4 < \alpha \leq \frac{2d}{3}$ and $d > 6$. If we i.i.d. initialize $w_r \sim \mathcal{N}(0, I)$, $a_r \sim \text{unif}\{-1, 1\}$ for $r \in [m]$, then with high probability at least $1 - \delta$ over the initialization, we have

$$L(t) \leq A(\alpha, d, \lambda_0) t^{-\alpha} L(0)$$

(4.6)

where $A(\alpha, d, \lambda_0)$ is a constant that only depends on $\alpha$, $d$ and $\lambda_0$.

We pause here to discuss the choice of $d$ in (4.1). In [59], the ‘magic constant’ $d$ has been extensively studied. When $d \geq 3$, the convergence rate is shown to be $O(t^{-\frac{2d}{3}})$. When $d < 3$, there exist counter-examples that fail the desired $O(1/t^2)$ convergence rate. We remark that we only need $d > 3$ to derive the convergence but we assume $d > 6$ only to guarantee the lazy training $w_r(t) \approx w_r(0)$.

From Theorem 3, NAG only converges at polynomial rate, in contrast to the linear convergence of HB and GD. This can be visualized as the linear pattern in Figure 2 (note the GD pattern is concave). Therefore, in the long run when $t$ is sufficiently large, NAG may be outperformed by GD. In addition, NAG and HB are well-known to have non-monotone loss dynamics, which is different than GD.

Figure 2: Logarithm MSE vs. logarithm epoch of NAG on MNIST. We observe that NAG shows polynomial decay in loss but converges faster than GD with learning rate $5 \times 10^{-5}$. Details of experiments are left in Appendix D.2.

4.1 Proof of Theorem 3

To prove Theorem 3, we use the same framework as in Section 3: given Lemma 3.1 and 3.2, we will prove Lemma 4.1 as an analogy to Lemma 3.3, but customized for NAG.

Lemma 4.1. Assume $0 \leq s \leq t$ and $\lambda_{\min}(H(s)) \geq \frac{\lambda_0}{2}$. Then we have $L(t) \leq \frac{C(\alpha, d)}{t^{\alpha}(\lambda_0/2)^{\frac{\alpha}{2}}} \tilde{L}(0)$ for $2 \leq \alpha \leq \frac{2}{3} d$ and some $C(\alpha, d)$ only depending on $\alpha$ and $d$. Furthermore, if $\alpha > 4$, we have

$$\|w_r(t) - w_r(0)\|_2 \leq R(\epsilon) := \frac{2\epsilon^{2 - \alpha/2}}{\alpha - 4} \sqrt{\frac{nC(\alpha, d) \tilde{L}(0)}{m(\lambda_0/2)^{\frac{\alpha}{2}} (d - \alpha/2 + 1)^2}} + \sqrt{2L(0)\epsilon}.$$
Proof. We define the Lyapunov function as in [59]

\[ V(t; \alpha, d) := t^\alpha \hat{L}(t) + \frac{(2d - \alpha)^2 t^{\alpha-2}}{8} \left\| \Delta_t + \frac{2t}{2d - \alpha} \hat{\Delta}_t \right\|^2 \]

and use the same loss \( L \) and pseudo-loss \( \hat{L} \) as before.

For \( d > 3 \) and \( 2 \leq \alpha \leq \frac{2d}{3} \), we apply from [59, Theorem 8], with some \( C(\alpha, d) \) only depending on \( \alpha \) and \( d \),

\[ \hat{L}(t) \leq \frac{C(\alpha, d)}{t^\alpha (\lambda_0/2)^{\frac{\alpha + 2}{2}}} L(0). \]

Leveraging \( \lambda_{\text{min}}(H) \geq \frac{\lambda_0}{2} \), we have \( \hat{L}(t) \geq \frac{\lambda_0}{2} L(t) \) and

\[ L(t) \leq \frac{2}{\lambda_0} \hat{L}(t) \leq \frac{C(\alpha, d)}{t^\alpha (\lambda_0/2)^{\frac{\alpha + 2}{2}}} L(0) \leq \frac{C(\alpha, d)}{t^\alpha (\lambda_0/2)^{\frac{\alpha + 2}{2}}} \hat{L}(0) \]

in which we denote \( A(\alpha, d, \lambda_0) = \frac{C(\alpha, d)}{(\lambda_0/2)^{\frac{\alpha + 2}{2}}} \). Since the weight dynamics is

\[ \ddot{w}_r(t) + \frac{d}{t} \dot{w}_r(t) + \frac{\partial f}{\partial w_r} (f - y) = 0, \]

multiplying both sides with \( t^d \), we obtain

\[ \frac{d}{dt} (t^d \dot{w}_r(t)) = -t^d \frac{\partial f}{\partial w_r} (f - y) = -\frac{1}{\sqrt{m}} t^d a_r \sum_i (f_i - y_i) x_i \mathbb{I}(w_r^\top x_i \geq 0) \]

which gives a close-form solution

\[ \dot{w}_r = -\frac{1}{t^d} \int_0^t \frac{1}{\sqrt{m}} s^d a_r \sum_i (f_i - y_i) x_i \mathbb{I}(w_r^\top x_i \geq 0) ds \]

whose norm satisfies

\[ \| \dot{w}_r \|_2 \leq \frac{1}{t^d \sqrt{m}} \int_0^t s^d \sum_i |f_i(s) - y_i| ds \]

\[ \leq \frac{1}{t^d \sqrt{m}} \int_0^t s^d \| f(s) - y \|_2 ds \]

\[ = \frac{1}{t^d \sqrt{m}} \int_0^t s^d \sqrt{L(s)} ds \]

\[ \leq \frac{1}{t^d \sqrt{m}} \frac{nC(\alpha, d) \hat{L}(0)}{m(\lambda_0/2)^{\frac{\alpha + 2}{2}}} \int_0^t s^{d-\alpha/2} ds \]

\[ = t^{1-\alpha/2} \left[ \frac{nC(\alpha, d) \hat{L}(0)}{m(\lambda_0/2)^{\frac{\alpha + 2}{2}} (d - \alpha/2 + 1)^2} \right]. \]
Next we bound the weight distance by breaking the integral into two pieces, for any $0 < \epsilon < t$:

$$\| \mathbf{w}_r(t) - \mathbf{w}_r(0) \|_2 \leq \int_0^t \| \mathbf{\dot{w}}_r(s) \|_2 \, ds = \int_0^t \| \mathbf{\dot{w}}_r(s) \|_2 \, ds + \int_t^\epsilon \| \mathbf{\dot{w}}_r(s) \|_2 \, ds$$

$$\leq 2e^{2-\alpha/2} \alpha - 4 \sqrt{\frac{nC(\alpha, d)\hat{L}(0)}{m(\lambda_0/2)^{\alpha/2} (d - \alpha/2 + 1)^2}} + \int_0^\epsilon \| \mathbf{\dot{w}}_r(s) \|_2 \, ds.$$

Now we need to bound $\| \mathbf{\dot{w}}_r(s) \|_2$ in $\int_0^\epsilon \| \mathbf{\dot{w}}_r(s) \|_2 \, ds$ with a time-independent upper bound, different than the previous $O(t^{1-\alpha/2})$ one. We achieve this goal by analyzing another Lyapunov function from [19].

$$E(t) = L(W(t), \alpha) + \frac{1}{2} \sum_r \mathbf{\dot{w}}_r(t)^\top \mathbf{\dot{w}}_r(t).$$

By simple differentiation, we see $E$ is decreasing in $t$ since $\dot{E}(t) = -\sum_r \frac{d}{2} \| \mathbf{\dot{w}}_r(t) \|^2_2 \leq 0$. This implies that

$$\frac{1}{2} \sum_r \mathbf{\dot{w}}_r(t)^\top \mathbf{\dot{w}}_r(t) \leq E(t) \leq E(0) = L(0).$$

Hence we obtain from $\| \mathbf{\dot{w}}_r(s) \|^2 \leq \sum_r \| \mathbf{\dot{w}}_r(s) \|^2$ that

$$\int_0^\epsilon \| \mathbf{\dot{w}}_r(s) \|_2 \, ds \leq \int_0^\epsilon \sqrt{\sum_r \| \mathbf{\dot{w}}_r(s) \|^2} \, ds \leq \sqrt{2L(0)\epsilon}.$$

Therefore, for any $\epsilon$ and $m$, we have

$$\| \mathbf{w}_r(t) - \mathbf{w}_r(0) \|_2 \leq R'(\epsilon) := \frac{2e^{2-\alpha/2}}{\alpha - 4} \sqrt{\frac{nC(\alpha, d)\hat{L}(0)}{m(\lambda_0/2)^{\alpha/2} (d - \alpha/2 + 1)^2}} + \sqrt{2L(0)\epsilon}.$$

Lastly, we give Lemma 4.2 in analogy to Lemma 3.4, in order to show that if $R'(\epsilon) < R$, then the conditions in Lemma 3.1 and Lemma 3.2 hold.

**Lemma 4.2.** If $R' < R$, then we have $\lambda_{\min}(H(t)) \geq \frac{1}{2}\lambda_0$, for all $r \in [m]$, $\| \mathbf{w}_r(t) - \mathbf{w}_r(0) \|_2 \leq R'$ and $L(t) \leq t^{-\alpha}A(\alpha, d, \lambda_0)\hat{L}(0)$, for $4 < \alpha \leq \frac{2d}{3}$ and $d > 6$.

The width requirement for $R' < R$ is equivalent to $\frac{2e^{2-\alpha/2}}{\alpha - 4} \sqrt{\frac{nC(\alpha, d)\hat{L}(0)}{m(\lambda_0/2)^{\alpha/2} (d - \alpha/2 + 1)^2}} + \sqrt{2L(0)\epsilon} < O(\frac{\lambda_0}{m^2})$ for a sufficiently small fixed $\epsilon > 0$. We show the details in Appendix A.2 that it suffices to use sufficiently large $m = \Omega \left( \frac{\lambda_0^{5\alpha/2-4}}{d \lambda_0^{2-3}} \right)$. We note this width lower bound is larger than the width required by GD in [22] and our HB analysis, suggesting smaller $\alpha$ or $d$ may be preferred for NAG (see Figure 3).
Figure 3: MSE loss with different width of the hidden layer on MNIST. We observe that NAG with larger \( d \) may require wider layer to converge at optimal rate. Here we fix the learning rate at \( 5 \times 10^{-5} \) and the dots represent minimum MSE for each case. The loss is averaged of 10 runs. Details of experiments are left in Appendix D.2.

5 Notable Extensions

The limiting ODE of different optimization algorithms gives rise to a general framework of analyzing the strongly-convex pseudo-loss \( \hat{L} \). We can further extend the analysis in some major directions: higher order ODE, higher order optimization algorithms and deeper neural networks.

5.1 Higher order momentum

We consider the convergence behavior of higher order ODE, resulting from using multiple momentums in GD, as an extension of HB.

\[
\mathbf{w}_r(k + 1) = \mathbf{w}_r(k) - \eta \frac{\partial L(W(k), \mathbf{a})}{\partial \mathbf{w}_r(k)} + \sum_{j \in [J]} \beta_j (\mathbf{w}_r(k - j + 1) - \mathbf{w}_r(k - j))
\]

which reduces to HB when \( J = 1 \) and to GD when \( J = 0 \). Consequently, the gradient flow is a \((J + 1)\)-th order ODE,

\[
\frac{d^{J+1}}{dt^{J+1}} \mathbf{w}_r(t) + \sum_{j \in [J]} b_j \frac{d^j}{dt^j} \mathbf{w}_r(t) + \frac{\partial L(W(t), \mathbf{a})}{\partial \mathbf{w}_r(t)} = 0.
\]

By similar argument as in [3,6], we have the higher order derivative \( \frac{\partial f}{\partial W_j} \) \text{ a.s.} = 0 for \( j > 1 \), hence the error dynamics follows the same form as the weight dynamics, except \( L \) is replaced by \( \hat{L} \). To see this, we have \( \frac{\partial f}{\partial W_j} \) \text{ a.s.} \( = \sum_r \frac{\partial f}{\partial w_r} \frac{d^j w_r(t)}{dt^j} \) and

\[
\frac{d^{J+1}}{dt^{J+1}} \Delta(t) + \sum_{j \in [J]} b_j \frac{d^j}{dt^j} \Delta(t) + \frac{\partial \hat{L}}{\partial \Delta(t)} = 0.
\]
To directly analyze this high order ODE is difficult. For the special case of $J = 2$, a second momentum has been shown to further accelerate the convergence than the first momentum \cite{48}, when the loss is a positive quadratic form. Empirically, we observe that, although $L$ is not convex nor quadratic, employing the second momentum leads to faster convergence as well.

![Figure 4: Logarithm MSE for optimization algorithms with different number of momentums on MNIST. We observe that the higher momentum method allows faster convergence rate than GD and HB. Details of experiments are left in Appendix D.3.](image)

5.2 Newton’s method

In this section we study the higher order optimization algorithms that use Hessian information. By the definition of Newton-Ralphson method, we have

$$w_r(k + 1) = w_r(k) - \nabla^2 L(W(k), a)^{-1}\nabla L(W(k), a)$$

in which $\nabla^2 L = \frac{\partial^2 L}{\partial w_r^2}$ and $\nabla L = \frac{\partial L}{\partial w_r}$. We observe by the chain rule (c.f. \cite{3.6}) that

$$\frac{\partial^2 L}{\partial w_r^2} = \left\langle \frac{\partial f}{\partial w_r}, \frac{\partial f}{\partial w_r} \right\rangle + \frac{\partial^2 f}{\partial w_r^2} (f - y) \text{ a.s.} = \left\langle \frac{\partial f}{\partial w_r}, \frac{\partial f}{\partial w_r} \right\rangle \in \mathbb{R}^{p \times p}.$$  

The corresponding gradient flow is then a first order ODE

$$\dot{w}_r = - \left( \left( \frac{\partial f}{\partial w_r} \right)^\top \frac{\partial f}{\partial w_r} \right)^{-1} \left( \frac{\partial f}{\partial w_r} \right)^\top (f - y)$$

The error dynamics can be obtained by left multiplying $\frac{\partial f}{\partial w_r}$ and summing over $r$. Denoting $R_r(t) := \frac{\partial f}{\partial w_r(t)} \in \mathbb{R}^{n \times p}$, we have

$$\dot{\Delta}(t) = - \sum_r R_r \left( R_r^\top R_r \right)^{-1} R_r^\top \Delta(t)$$
In order to guarantee the linear convergence, we need the sum of matrices, which we refer to as \( M(t) = \sum_r R_r (R_r^T R_r)^{-1} R_r^T \in \mathbb{R}^{n \times n} \), to be positive definite for all \( t \). Notice \( M(t) \) is clearly positive semi-definite. It suffices to show \( v^T \left[ \sum_r R_r (R_r^T R_r)^{-1} R_r^T \right] v > 0 \), for any non-zero vector \( v \). In fact, we have

\[
v^T \left[ \sum_r R_r (R_r^T R_r)^{-1} R_r^T \right] v = \sum_r \frac{1}{\lambda_{\text{max}}(R_r R_r^T)} \|R_r^T v\|^2 \geq \sum_r \frac{1}{\lambda_{\text{max}}(R_r R_r^T)} \|R_r^T v\|^2 \geq \frac{1}{\max_r \lambda_{\text{max}}(R_r R_r^T)} \sum_r \|R_r^T v\|^2 = \frac{1}{\max_r \lambda_{\text{max}}(R_r R_r^T)} v^T H(t) v
\]

which is positive if \( H(t) \) is always positive definite. In other words, the linear convergence factor \( \lambda_{\text{min}}(M) \) is larger than \( \lambda_{\text{min}}(H)/\max_r \lambda_{\text{max}}(R_r R_r^T) \). We notice that \( \max_r \lambda_{\text{max}}(R_r R_r^T) \ll 1 \) since \( \lambda_{\text{max}}(R_r R_r^T) = \text{tr}(R_r R_r^T) = \sum_r \frac{1}{m} \|w_r^{(l)} x_i \geq 0 \leq \frac{m}{m} \) from [20] and if we assume \( m \) is of polynomial order of \( n \), as in previous theorems. This implies a significant boost of linear convergence rate compared to GD for large \( m \), i.e. for over-parameterized neural networks.

### 5.3 Multi-layer Training

Though we do not dive into the detailed proof of extending our main theorem to multi-layer neural network, including training both layers of the two-layer neural network and deep neural networks, we provide a sketch proof direction as follows:

On high level, we can write the training dynamics for the deep fully-connected neural networks as

\[
x_r^{(l)} = \frac{1}{\sqrt{m}} \sigma \left( (w_r^{(l)})^T x^{(l-1)} \right)
\]

\[
f(x; W, a) = a^T x^L
\]

in which the layer index \( l \in [L-1] \), input \( x^{(0)} = x \), the post-activation \( x_r^{(l)} \) corresponds to the \( r \)-th hidden neuron in the \( l \)-th layer and each layer has \( m \) hidden neurons, i.e. \( r \in [m] \).

We denote the union of all weights as \( W = \{ w_r^{(1)}, \ldots, w_r^{(L-1)}, a \} \). Similar to (2.2)-(2.4), we have

\[
\dot{\Delta}(t) + b(t) \dot{\Delta}(t) + H(t) \Delta(t) = 0
\]

where \( b(t) \) depends on different optimization algorithms. Here the NTK is \( H_{\text{multi}}(t) = \sum_l H_l(t) + H_a(t) \) with \( H_l(t) = \sum_r \frac{\partial f(t)}{\partial w_r^{(l)}} \left( \frac{\partial f(t)}{\partial w_r^{(l)}} \right)^T \) and \( H_a(t) = \frac{\partial f(t)}{\partial a(t)} \left( \frac{\partial f(t)}{\partial a(t)} \right)^T \). Clearly \( H_l \) and \( H_a \) are positive semi-definite. Therefore it suffices to show there exists one \( l \in [L-1] \) that is positive definite. In our two-layer analysis, we show the Gram matrix corresponding to the last (and the first) hidden layer is positive definite. We note that [21] has also shown \( H_{L-1} \) is positive definite for GD and for deep fully-connected neural networks. We believe similar analysis applies to other optimization algorithms such as HB and NAG.
6 Discussion

In this paper, we extend the convergence analysis of over-parameterized neural networks to different accelerated optimization algorithms, including the Heavy Ball method (HB) and the Nesterov accelerated gradient descent (NAG). Our analysis is based on the neural tangent kernel (NTK) which characterizes the training dynamics as ODEs known as the gradient flows. We observe that, for piecewise linear activation functions (e.g. ReLU, Leaky ReLU [42] and maxout [29, 32]), the weight dynamics takes the same form as the error dynamics (for example, (3.3) and (3.4)), with the only difference lying in the losses. To see this, we recall \( \frac{\partial^2 f}{\partial w_r \partial w_l} \equiv 0 \) for piecewise linear activations. In particular, the loss in the error dynamics is strongly-convex, leading to linear convergence of HB (and GD) and polynomial decay of NAG. We emphasize that by constructing the strongly-convex loss \( \hat{L} \), we can easily borrow the rich results from the convex optimization world to analyze the convergence of neural networks on non-convex loss. We remark that instead of using the Gronwall inequality, as in the case of GD [22], we use the Lyapunov function, which is a common and traditional tool in solving ODE with convex loss. In fact, the Gronwall inequality generally does not work on second or higher order ODE.

A major extension of our one-layer training process will be to train all layers in deep neural networks, which has been well-established for GD in [3, 21] for various types of neural networks such as RNN, CNN, ResNet, Graph neural networks (GNN) and Generative Adversarial networks (GAN). Since the main focus of this work is on the optimization algorithms instead of neural network architectures, we do not over-complicate our proof by exploring deeper learning (including two-layer training) and other architectures. For similar reasons, we claim the discrete time convergence analysis of the HB and NAG is similar to their continuous time counter-parts and can be derived within our framework of proofs, but we do not try to present the rigorous theorems in this paper.

Our analysis may further extend to more optimization algorithms. Unlike GD, HB and NAG, many popular optimization algorithms adopt adaptive learning rates and demonstrate impressive performance. Examples include AdaGrad [23], AdaDelta [63], RMSprop [33], Adam [35], AdaFom [16], DIN [5] and especially their variants with momentums and mini-batches. Notably, optimization algorithms with adaptive learning rates can correspond to a system of limiting ODEs, instead of a single ODE. In [58], the following systems of ODEs characterize the evolution of Adam, AdaFom, HB and NAG with different functions \( (h, \gamma, p, q) \) on the left and the evolution of AdaGrad and RMSprop without a momentum term \( m_r(t) \) on the right:

\[
\begin{align*}
\dot{w}_r(t) &= -\frac{\dot{m}_r(t)}{\sqrt{v_r(t)} + \varepsilon} \\
\dot{m}_r(t) &= h(t) \frac{\partial L}{\partial w_r(t)} - \gamma(t) m_r(t) \\
\dot{v}_r(t) &= p(t) \left[ \frac{\partial L}{\partial w_r(t)} \right]^2 - q(t) v_r(t)
\end{align*}
\]

or

\[
\begin{align*}
\dot{w}_r(t) &= -\frac{\partial L}{\partial w_r(t)} / \sqrt{v_r(t) + \varepsilon} \\
\dot{v}_r(t) &= p(t) \left[ \frac{\partial L}{\partial w_r(t)} \right]^2 - q(t) v_r(t)
\end{align*}
\]

Interestingly, we observe that the error dynamics again follows a similar form of the weight dynamics. Suppose we consider the memory term \( v_r(t) \in \mathbb{R}^p \) with identical entries across \( r \), i.e. all weights share the same adaptive learning rate. These optimizers are still adaptive to the training dynamics though not in a per-parameter sense. Then we can treat \( v_r(t) \) as a scalar \( v(t) \). By multiplying \( \frac{\partial f}{\partial w_r} \) and sum over \( r \), the error dynamics for adaptive optimization
algorithms will be

\[
\begin{cases}
\hat{\Delta}(t) = -Q(t) / \sqrt{v(t)} + \varepsilon \\
\dot{Q}(t) = h(t) \frac{\partial \hat{L}}{\partial \Delta(t)} - \gamma(t) Q(t)
\end{cases}
\]

or

\[\hat{\Delta}(t) = - \frac{\partial \hat{L}}{\partial \Delta(t)} / \sqrt{v(t)} + \varepsilon\]

in which \(Q(t) := \sum_r \frac{\partial f}{\partial w_r} m_r(t)\). It would be desirable to analyze these adaptive optimization algorithms in future works, though the convergence analysis can be more difficult than in this work and require more advanced tools in Lyapunov function and ODE theory.
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A Deriving Width from $R' < R$

In this section we derive the width requirement for our main theorems. We slightly abuse the notation of $\alpha$ here: For HB analysis, $\alpha := \sqrt{\lambda_0/2}$. For NAG analysis, $\alpha$ is a constant in $[4, 2d/3]$.

A.1 Width requirement in Theorem 2 (HB)

To guarantee $R' < R$, we need $\sqrt{32 n \hat{L}(0)} < O\left(\frac{2 \lambda_0}{\delta_0^2} n \frac{\lambda_0}{\delta_0} \cdot \hat{L}(0)\right)$. Since $\lambda_{\text{min}}(H(0)) > \lambda_0/2$, we have $\hat{L} > \frac{1}{\delta_0^2} L(0)$ and we can bound $L(0)$ using Markov’s inequality: with probability at least $1 - \delta$, we obtain $\hat{L} = O\left(\frac{n}{\delta}\right)$, because $E[L(0)^2] = \sum_{i=1}^{n} (y_i^2 + y_i E[f(W(0), a, x_i)] + E[f(W(0), a, x_i)^2]) = \sum_{i=1}^{n} (y_i^2 + 1) = O(n)$.

Therefore

$$m = \Omega\left(\frac{n^4}{\delta^2 \lambda_0^4} \cdot \frac{n \lambda_0}{\delta} \lambda_0^6\right) = \Omega\left(\frac{n^6}{\delta^3 \lambda_0^5}\right).$$

A.2 Width requirement in Theorem 3 (NAG)

To guarantee $R' < R$, we need $2^{\alpha-2/\alpha-4} \sqrt{\frac{nC(\alpha, d)L(0)}{m(\lambda_0/2)^{\alpha-4} (d-\alpha/2+1)^2}} + \sqrt{2L(0)} \epsilon < O\left(\frac{4 \lambda_0}{\delta_0^2}\right)$. Choose small enough $\epsilon$ such that $\sqrt{2L(0)} \epsilon < R/2$. This is equivalent to set $\epsilon = O\left(\frac{4 \lambda_0}{\delta_0^2}\right)$ since $L(0) = O(n/\delta)$. Then we need $2^{\alpha-2/\alpha-4} \sqrt{\frac{nC(\alpha, d)L(0)}{m(\lambda_0/2)^{\alpha-4} (d-\alpha/2+1)^2}} < R/2$. Ignoring constant terms, this is equivalent to $\epsilon^2 = O\left(\frac{4 \lambda_0}{\delta_0^2}\right)$ and further to $m = \Omega\left(\frac{\epsilon^{\alpha-2} n^6}{\lambda_0^{2\alpha-4} \delta_0^3} \cdot \hat{L}(0)\right)$. Similar to the analysis in the previous section, we have $\hat{L}(0) = O(n \lambda_0/\delta)$ and therefore

$$m = \Omega\left(\frac{n^{5 \alpha/2-4}}{\delta^{3 \alpha/2-3} \lambda_0^{3 \alpha/2-2}}\right).$$

Notice that as $\alpha \to 4$, the width requirement tends to the same width as for GD and HB. Moreover, the width is increasing in $\alpha$.

B The derivative of higher momentum

Here we derive the iterative term for second-order momentum for implementation. Recall that for second-order momentum, $[J] = \{1, 2\}$. Hence,

$$w_r(t + 1) = w_r(t) - \eta \frac{\partial L(w_r(t), a)}{\partial w_r(t)} + \beta_1(w_r(t) - w_r(t - 1)) + \beta_2(w_r(t - 1) - w_r(t - 2))$$
Denoting \( \frac{\partial L(w_r(t), a)}{\partial w_r(t)} \) as \( g(t) \) gives the following term:
\[
w_r(t + 1) = w_r(t) - \eta g(t) + \beta_1 (w_r(t) - w_r(t - 1)) + \beta_2 (w_r(t - 1) - w_r(t - 2))
\]

Introducing two new variables \( v, q \) and given an objective loss function \( L \) to be minimized, classical momentum is given by:
\[
w_r(t + 1) = w_r(t) - \eta v(t + 1)
\]
\[
v(t + 1) = av(t) + q(t + 1)
\]
\[
q(t + 1) = bq(t) + g(t)
\]

where \( a = \frac{1}{2}(\beta_1 + \sqrt{\beta_1^2 + 4\beta_2}) \) and \( b = \frac{1}{2}(\beta_1 + \sqrt{\beta_1^2 - 4\beta_2}) \). Note that when \( \beta_2 = 0 \), the above momentum is the momentum of heavy ball. And when \( \beta_1 = 0, \beta_2 = 0 \), it can recover gradient descent.

C Proof of Lemma 3.4 and 4.2

This proof is almost identical to [22, Lemma 3.4] and is adapted to here for the completeness of our paper.

Suppose the conclusion does not hold for at time \( t \). Then we split the analysis into two cases:
1. there exists \( r \in [m] \) such that \( \|w_r(t) - w_r(0)\|_2 \geq R' \); 2. \( L(t) \geq \frac{4}{\lambda_0} \exp(-\sqrt{\lambda_0/2} t) \hat{L}(0) \).

For case (1), if we are proving Lemma 3.3 or \( L(t) \leq A(\alpha, d, \lambda_0) t^{-\alpha} \hat{L}(0) \) if we are proving Lemma 4.1. We know there exists \( s \leq t \) such that \( \lambda_{\min}(H(s)) < \frac{1}{2} \lambda_0 \). However, Lemma 3.2 shows that there exists a \( t_0 \) with
\[
t_0 = \inf \left\{ t > 0 : \max_{r \in [m]} \|w_r(t) - w_r(0)\|_2^2 \geq R \right\}
\]

Consequently, there exists \( r \in [m] \) that \( \|w_r(t_0) - w_r(0)\|_2 = R \). Applying Lemma 3.2, we know that \( H(t') \geq \frac{1}{2} \lambda_0 \) for \( t' \leq t_0 \). However, by Lemma 3.3/4.1 we know \( \|w_r(t_0) - w_r(t)\|_2 < R' < R \), a contradiction.

For case (2), at time \( t \), \( \lambda_{\min}(H(t)) < \frac{1}{2} \lambda_0 \) we know there exists
\[
t_0 = \inf \left\{ t \geq 0 : \max_{r \in [m]} \|w_r(t) - w_r(0)\|_2^2 \geq R \right\}
\]

The rest of the proof is the same as the previous case.

D Experiment

The MNIST dataset [37] is a dataset of handwritten digits ranging from 0 to 9. It contains 60,000 training images and 10,000 test images. Each image is in \( 28 \times 28 \) gray-scale. We train the two-layer neural networks with random initialization: \( w_r \) (the weight in the first layer) is initialized with distribution \( \mathcal{N}(0, I) \) and \( a_r \) (the weight in the second layer) is initialized with distribution \( \text{unif}\{-1, 1\} \). We randomly take 600 subsamples out of the original training dataset, in order to run full-batch gradient descents within limited GPU memory.
D.1 Experiment of Heavy Ball (HB)

This subsection corresponds to Figure 1. The neural network is trained in 5000 steps with hidden neurons in the two-layer neural network is 3000. We use three different momentum term $\beta = 0, 0.2, 0.5, 0.8$ with learning rate $10^{-4}$. When $\beta = 0$, the HB reduces to GD. We take the log of MSE in the y-axis. The constant slope in figures depicts the linear convergence rate.

D.2 Experiment of Nesterov Accelerated Gradient (NAG)

The basic setting of Figure 2 is the same as D.1 except we replace the momentum term with "nesterov term" $d$, which are 2, 3, 6, 8 respectively. We take log on both the time/step size as well as the MSE loss to show the polynomial decay of NAG. In Figure 3 the learning rate is fixed as $5 \times 10^{-5}$ while width ranges from 1000 to 9000. The experiment is run for ten times using different seeds for random initialization and we record the loss at epoch 200 for every $d$ and width.

D.3 Experiment of Higher Momentum

In Figure 4 we take $\beta_1 = 0, 0.2$ and $\beta_2$ varies from 0, 0.2, 0.5. Here $\beta_2 = 0$ recovers the Heavy Ball (HB) and $\beta_1 = 0$ recovers the Gradient Descent (GD). The total number of epochs, number of hidden neurons and learning rate are the same as D.1 We take log of MSE in the y-axis along with epochs in the x-axis.