Implicit bias of deep linear networks in the large learning rate phase

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Abstract

Correctly choosing a learning rate (scheme) for gradient-based optimization is vital in deep learning since different learning rates may lead to considerable differences in optimization and generalization. As found by Lewkowycz et al. [27] recently, there is a learning rate phase with large stepsize named catapult phase, where the loss grows at the early stage of training, and optimization eventually converges to a flatter minimum with better generalization. While this phenomenon is valid for deep neural networks with mean squared loss, it is an open question whether logistic (cross-entropy) loss still has a catapult phase and enjoys better generalization ability. This work answers this question by studying deep linear networks with logistic loss. We find that the large learning rate phase is closely related to the separability of data. The non-separable data results in the catapult phase, and thus flatter minimum can be achieved in this learning rate phase. We demonstrate empirically that this interpretation can be applied to real settings on MNIST and CIFAR10 datasets with the fact that the optimal performance is often found in this large learning rate phase.

1 Introduction

Deep neural networks have been achieving a variety of successes in both supervised and unsupervised learning. A theoretical understanding of the mechanism behind deep learning’s achievement is a long-term goal pursued by researchers. Remarkably, recent progress in deep learning theory shows that over-parameterized networks are capable of achieving very low, even zero loss through gradient descent based optimization [17, 8, 10, 34].

Meanwhile, these over-parameterized networks can generalize well to the test set, which is known as the double descent phenomenon [33]. How can over-parameterized networks survive from the over-fitting problem given that model parameters are much more than the size of data? This is a largely open problem, and one promising answer is implicit bias [40] or regularization [34]. In this direction, a large family of works working on the exponential tailed loss such as logistic (cross-entropy) and exponential loss has reported a strong regularization connected with maximum margin [40, 11, 20, 31, 50].

However, all theoretical results regarding implicit bias require that the learning rate should be sufficiently small. Thus we still have a limited understanding of what happens when the learning rate

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goes beyond the small learning rate regime. Besides, it is becoming more significant to study the large learning rate in deep learning since adopting an annealing learning scheme that starts from a large learning rate often achieves better performance. [13, 43, 28, 25]. To this end, Lewkowycz et al. [27] found that a distinct phenomenon that the local curvature of the loss landscape drops significantly in the large learning rate phase and thus typically can obtain the best performance. This learning rate phase is called catapult phase and whether it can be extended to logistic loss remains unclear.

To fill this gap, we address the large learning rate phase problem for one hidden layer linear network with a logistic (exponential) loss. By studying the learning rate partition problem on the linearly separable and non-separable dataset, we find that richer partitions on the non-separable case, which is similar to mean squared loss case [27]. We introduce the learning rate phase partition here (i) lazy phase $\eta < \eta_0$, when the learning rate is small, the dynamics of neural networks its linearized dynamics regime, where model converges to a nearby point in parameter space which is call lazy training [17, 4, 41, 15, 3, 10]. (ii) catapult phase $\eta_0 < \eta < \eta_1$, the loss grows at beginning and then drops until converges to the solution with a flatter minimum. (iii) divergent phase $\eta > \eta_1$, the loss diverges and the model does not train. For details regarding this partition, please refer to [27]. Finally, we summarize our contribution as follows:

- We find that the learning rate partition is associated with the separability property of the dataset. When the dataset is linearly separable, there will not be a catapult phase. For the non-separable dataset, the catapult phase emerges.
- Our analysis ranges from linear predictor to one hidden layer network. By comparing the convex (linear predictor) and non-convex (one hidden layer network) optimization in terms of learning rate, we show that the catapult phase is a unique phenomenon of non-convex optimization.
- We find that in practical classification tasks, the best generalization results tend to occur in the catapult phase. Given the fact that the infinite-width analysis does not explain the practically observed power of deep learning [2, 8]. Our result can be used to partially fill the gap between lazy training and real power of deep learning.

2 Related Work

Implicit bias of gradient methods. Since the seminal work from [40], implicit bias has led to a fruitful line of research. Works along this line have treated linear predictors [11, 20]; deep linear networks with a single output [32, 12, 19] and multiple outputs [38]; homogeneous networks (including ReLU, max pooling activation) [31, 30, 21]; ultra wide networks [7, 37]; matrix factorization [39]. However, these studies all focus on the gradient flow (infinitesimal learning rate) or small learning rate regime. Our work addresses the problem above a critical learning rate in which the theoretical guarantee for maximum margin will vanish, and can seen as a form of implicit bias.

Neural tangent kernel. Recently, we have witnessed exciting theoretical developments in understanding the optimization of ultra wide networks, known as the neural tangent kernel (NTK) [17, 4, 41, 15, 3, 10, 44]. It is shown that in the infinite-width limit, NTK converges to an explicit limiting kernel, and it stays constant during training. Further, Lee et al. [26] show that gradient descent dynamics of the original neural network falls into its linearized dynamics regime in the NTK regime. In addition, NTK has been verified in various architecture such as orthogonal initialization [16], convolutions [4, 29], graph neural networks [9], attention [14], batch normalization [18] and see [42] for a summary. The constant property of neural tangent kernel during training can be regarded as a special case of the implicit bias, and importantly, it is only true in the small learning rate regime. The neural tangent kernel varies with training step at large learning rate, and our analysis relies highly on this term.

Large learning rate and logistic loss. A large learning rate with SGD training is often set initially to achieve good performance empirically in deep learning [24, 13, 43]. Existing theoretical explanation of the benefit of the large learning rate contributes to two classes. One is that a large learning rate with SGD leads to flat minima [23, 22, 27] and the other is that the large learning rate acts as a regularizer [28]. Especially, Lewkowycz et al. [27] find a large learning rate phase can result in flatter minima without the help of SGD for mean squared loss. In this work, we ask whether large learning rate still
has this advantage for logistic loss. We expect this loss function to have a different outcome because the logistic loss is sensitive to the separable property of the data and the loss surface is quite different from that of MSE. For example, it is shown that gradient descent can learn less over-parameterized neural networks with logistic loss than mean squared loss based on separability [36].

3 Background

3.1 Setup

Consider a dataset \( \{x_i, y_i\}_{i=1}^{n} \), with inputs \( x_i \in \mathbb{R}^d \) and binary labels \( y_i \in \{-1, 1\} \). The risk of classification task follows the form,

\[
L = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i)y_i),
\]

where \( f(x_i) \) is the output of network regarding the input \( x_i \), and \( \ell \) is the loss. In this work, we study two exponential tail losses which are exponential loss \( \ell_{\text{exp}}(u) = \exp(-u) \) and logistic loss \( \ell_{\text{log}}(u) = \log(1 + \exp(-u)) \). The reason we look at these two loss together is that they show the same phenomenon under gradient descent on a linearly separable data set [40]. We adopt gradient descent (GD) updates with learning rate \( \eta \) to minimize empirical risk,

\[
w(t+1) = w(t) - \eta \nabla L(w(t)) = w(t) - \eta \sum_{i=1}^{n} \ell'(f(x_i)y_i).
\]

3.2 Problem structure

Before analyzing the dynamics of gradient descent on deep linear networks with logistic and exponential loss, we consider a simpler setting with only one layer network (no hidden layer). Since the loss surface and corresponding dynamics of gradient descent on linearly separable data and non-separable data are quite different, we first define the two data classes.

**Assumption 1.** The dataset is linearly separable, i.e. there exists a separator \( w^*_\star \) such that \( \forall i : w^*_\star^T x_i y_i > 0 \).

**Assumption 2.** The dataset is non-separable separable, i.e. there is no separator \( w^*_\star \) such that \( \forall i : w^*_\star^T x_i y_i > 0 \).

We construct our initial understanding of the relationship between loss surface and dynamics with different learning rate with logistic and experiential loss regarding the two classes of data throng the following proposition,

**Proposition 1.** For a linear predictor \( f = w^T x \), along with a loss \( \ell \in \{\ell_{\text{exp}}, \ell_{\text{log}}\} \).

1. Under Assumption [7] the empirical loss is \( \beta \)-smooth. Then the gradient descent with constant learning rate \( \eta < \frac{2}{\beta} \) never increase the risk, and empirical loss will converge to zero:

\[
L(w(t+1)) - L(w(t)) \leq 0, \quad \lim_{t \to \infty} L(w(t)) = 0, \quad \text{with} \quad \eta < \frac{2}{\beta},
\]

2. Under Assumption [2] the empirical loss is \( \beta \)-smooth and \( \alpha \)-strongly convex, where \( \alpha \leq \beta \). Then the gradient descent with a constant learning rate \( \eta < \frac{2}{\alpha} \) never increases the risk, and empirical loss will converge to a global minimum. On the other hand, the gradient descent with a constant learning rate \( \eta > \frac{2}{\alpha} \) never decrease the risk, and empirical loss will explode or saturate:

\[
L(w(t+1)) - L(w(t)) \leq 0, \quad \lim_{t \to \infty} L(w(t)) = G_0, \quad \text{with} \quad \eta < \frac{2}{\beta}
\]

\[
L(w(t+1)) - L(w(t)) \geq 0, \quad \lim_{t \to \infty} L(w(t)) = G_1, \quad \text{with} \quad \eta > \frac{2}{\alpha}
\]

where \( G_0 \) is the value of global minimum while \( G_1 = \infty \) for exploding situation or \( G_0 < G_1 < \infty \) when saturating.
Remark. In this proposition, we show the difference between the loss surface of two data classes.

(i) For linear separable data, the loss surface is smooth convex and the global minimum is at infinity. The implicit bias of gradient descent with a small enough learning rate in this phase has been studied by [40]. They show the predictor converges to the direction of the max-margin (hard margin SVM) solution, which implies the gradient descent method itself will find a proper solution instead of picking up a random solver. However, if one increases the learning rate until it exceeds $\eta < \frac{2}{\beta}$ for linearly separable data, then the result of converge to maximum margin will not be guaranteed, though it will still converge to global minimum.

(ii) On the other hand, the loss is strongly convex and the global minimum is finite for non-separable data. In this case, we can rigorously show that the large learning rate will lead to loss exploding or saturating.

4 Theoretical results

4.1 linear predictor

It is known that the Hessian of the logistic or exponential loss is non-constant, which means that indicators of convexity i.e. $\alpha$ and $\beta$ can be approximated differently at different positions. Despite this difficulty, we can obtain more concrete results with different learning rate for linear predictor. To theoretically investigate this problem, we consider the degeneracy assumption:

Assumption 3. The dataset contains two data points where they have same feature and opposite label, that is

$$(x_1 = 1, y_1 = 1) \text{ and } (x_2 = 1, y_2 = -1).$$

We call this assumption the degeneracy assumption since the position of data from opposite label degenerate. Without loss of generality, we simplify the dimension of data and fix the position of the feature. Note that this condition can be seen as a special case of non-separable data. There is a work theoretically characterizing general non-separable data [20], and we leave the analysis of this setting for the large learning rate to future work.

The following theorem consider the local geometry of loss surface in terms of learning rate thanks to the symmetry provided by degeneracy assumption and thus can construct the exact dynamics of empirical risk with respect to the whole learning rate regime.

Theorem 1. For a linear predictor $f = w^T x$ equipped with exponential (logistic) loss under assumption [3] there is a critical learning rate that separates the whole learning rate space into two (three) regions, which is depends on the initial weight. The critical learning rate satisfies

$$L'(w(0)) = -L'(w(0) - \eta_{\text{critical}} L'(w(0))),$$

where $w(0)$ is the initial weight. Moreover,

1. For exponential loss, the gradient descent process with a constant learning rate $\eta < \eta_{\text{critical}}$ never increases loss, and the empirical loss will converge to the global minimum. On the other hand, the gradient descent process with learning rate $\eta = \eta_{\text{critical}}$ will oscillate. Finally, when the learning rate $\eta > \eta_{\text{critical}}$, the training process never decreases the loss and the empirical loss will explode to infinity:

$$L(w(t+1)) - L(w(t)) < 0, \quad \lim_{t \to \infty} L(w(t)) = 1, \quad \text{with } \eta < \eta_{\text{critical}},$$

$$L(w(t+1)) - L(w(t)) = 0, \quad \lim_{t \to \infty} L(w(t)) = L(w(0)), \quad \text{with } \eta = \eta_{\text{critical}},$$

$$L(w(t+1)) - L(w(t)) > 0, \quad \lim_{t \to \infty} L(w(t)) = \infty, \quad \text{with } \eta > \eta_{\text{critical}}.$$

2. For logistic loss, the critical learning rate $\eta_{\text{critical}} > 8$. The gradient descent process with a constant learning rate $\eta < 8$ never increases the loss and the empirical loss will converge to the global minimum. On the other hand, the loss along the gradient descent process with a learning rate $8 \leq \eta < \eta_{\text{critical}}$ will not converge to global minimum but oscillate. Finally,
We successfully construct the dynamics and the ending of gradient descent for logistic and exponential loss with respect to different learning rate regimes. Due to the difference in the monotonicity of the loss function, the results are very different. For exponential loss, the function $L'(w(t))/w(t)$ is monotonically increasing from the origin. While the function $L'(w(t))/w(t)$ is monotonically decreasing for logistic loss. We demonstrate the gradient descent dynamics with the degenerate and non-separable case through the following example.

**Example 1.** Consider optimizing $L(w)$ with dataset $\{(x_1 = 1, y_1 = 1) \text{ and } (x_2 = 1, y_2 = -1)\}$ and exponential (logistic) loss using gradient descent with constant learning rate. Figure 1(a)(c) show how different choices of learning rate $\eta$ change the dynamics of training loss.

**Example 2.** Consider optimizing $L(w)$ with dataset $\{(x_1 = 1, y_1 = 1), \ (x_2 = 2, y_2 = -1) \text{ and } (x_3 = -1, y_3 = 1)\}$ and exponential (logistic) loss using gradient descent with constant learning rate. Figure 1(b)(d) show how different choices of learning rate $\eta$ change the dynamics of training loss. The dataset considered here is an example of a non-separable case, and the dynamics of loss behave similarly to those with Example 1.

**Remark.** We use this example to show that our theoretical results on the degenerate case can be extended to the general non-separable dataset empirically.

### 4.2 Two layer linear network

To investigate the relationship between the dynamics of gradient descent with learning rate for deep linear networks, we consider a two-layer linear network with only one hidden layer, and the information propagation in this network is governed by,

$$f(x_i) = m^{-1/2}w^{(2)}w^{(1)}x_i,$$

where $m$ is the width, i.e. number of neurons in the hidden layer, $w^{(1)} \in \mathbb{R}^{m \times d}$ and $w^{(2)} \in \mathbb{R}^m$ are the parameters of model. Taking the exponential loss as an example, the gradient descent equations
at training step $t$ are,

\[
\begin{align*}
  w_{ij}^{(1)}(t + 1) &= w_{ij}^{(1)}(t) - \frac{\eta}{m} \frac{x_j \exp x_i}{2} \left[ -e^{-y_0 f(x_\alpha)} w_{ij}^{(2)}(t) x_{ja} y_\alpha \right], \\
  w_{ij}^{(2)}(t + 1) &= w_{ij}^{(2)}(t) - \frac{\eta}{m} \frac{x_j \exp x_i}{2} \left[ -e^{-y_0 f(x_\alpha)} w_{ij}^{(1)}(t) x_{ja} y_\alpha \right],
\end{align*}
\]  

(4)

where we use the Einstein summation agreement to simplify the expression and will take this agreement in the following derivation.

Before deriving the update equation for the output, we introduce the neural tangent kernel, an essential element for the evolution of output function. The neural tangent kernel (NTK) is originated from [17] and formulated as,

\[
\Theta_{\alpha\beta} = \frac{1}{m} \sum_{p=1}^{P} \left( \frac{\partial f(x_\alpha)}{\partial \theta_p} \frac{\partial f(x_\beta)}{\partial \theta_p} \right),
\]

(5)

where $P$ is the number of parameters. For a two-layer linear neural network, the NTK can be written as,

\[
\Theta_{\alpha\beta} = \frac{1}{mn} \left( (w_{ij}^{(1)} x_{ja})(w_{ij}^{(1)} x_{ja}) + (w_{ij}^{(2)})^2 (x_{ja} x_{ja}) \right).
\]

(6)

here we use normalized NTK which is divided by the number of samples $n$. Under the degeneracy assumption the loss becomes $L = \cosh(m^{-1/2}w^{(2)}w^{(1)})$. Then the equation 4 reduces to

\[
\begin{align*}
  w_{ij}^{(1)}(t + 1) &= w_{ij}^{(1)}(t) - \frac{\eta}{m} \frac{x_j \exp x_i}{2} \left[ -e^{-y_0 f(x_\alpha)} w_{ij}^{(2)}(t) \sinh(m^{-1/2}w^{(2)}(t)w^{(1)}(t)), \\
  w_{ij}^{(2)}(t + 1) &= w_{ij}^{(2)}(t) - \frac{\eta}{m} \frac{x_j \exp x_i}{2} \left[ -e^{-y_0 f(x_\alpha)} w_{ij}^{(1)}(t) \sinh(m^{-1/2}w^{(2)}(t)w^{(1)}(t)).
\end{align*}
\]

(7)

We care about two quantities, the output function $f(t)$ and the eigenvalue of neural tangent kernel $\lambda(t)$, which are both scalars in our simplified setting:

\[
\begin{align*}
  f(t + 1) &= f(t) - \eta \lambda(t) \tilde{f}\text{exp}(t) + \frac{\eta^2}{m} f(t) \tilde{f}\text{exp}^2(t), \\
  \lambda(t + 1) &= \lambda(t) - \frac{4\eta}{m} f(t) \tilde{f}\text{log}(t) + \frac{\eta^2}{m} \lambda^2 \tilde{f}\text{exp}(t).
\end{align*}
\]

(8)

where $\tilde{f}\text{exp}(t) := \sinh(f_t)$ while $\tilde{f}\text{log}(t) := \frac{\sinh(f_t)}{1 + \cosh(f_t)}$ for logistic loss.

In the introduction section, we have introduced the catapult phase where the loss grows at the beginning and then drops until converges to a global minimum. In the following theorem, we show that the catapult phase exist thanks to the non-separability of the degenerate data.

**Theorem 2.** Under appropriate initialization and assumption there exists a catapult phase for both the exponential and logistic loss. More precisely, when $\eta$ belongs to this phase, the output function $f(t)$ and the eigenvalue of NTK $\lambda(t)$ update in the following way:

1. $L(t)$ keeps increasing when $t < T$.
2. After the $T$ step and its successors, the loss decreases, which is equivalent to:

   \[ |f(T + 1)| > |f(T + 2)| \geq |f(T + 3)| \geq \ldots. \]

3. The eigenvalue of NTK keeps dropping after the $T$ steps:

   \[ \lambda(T + 1) > \lambda(T + 2) \geq \lambda(T + 3) \geq \ldots. \]

Moreover, we have the inverse relation between the learning rate and the final eigenvalue of NTK:

\[ \lambda(\infty) \leq \lim_{t \to \infty} \frac{4f(t)}{\eta f\text{exp}(t)} \text{ with exponential loss, or } \lambda(\infty) \leq \lim_{t \to \infty} \frac{4f(t)}{\eta f\text{log}(t)} \text{ with logistic loss.} \]

**Remark.** For mean squared loss, the catapult phase can be found in both linearly separable data and non-separable data with deep linear networks. While exponential and logistic loss have a requirement that data should be non-separable.
We demonstrate that catapult phase can be found in degenerate and general non-separable case through the following examples. The weights matrix is initialized by Gaussian distribution, i.e. $w^{(1)}, w^{(2)} \sim N(0, \sigma^2_w)$. For exponential loss, we adopt the setting of $\sigma^2_w = 0.5$ and $m = 1000$ while we set $\sigma^2_w = 1.0$ and $m = 100$ for logistic loss.

**Example 3.** Consider optimizing $\mathcal{L}(w)$ using one hidden layer linear networks with dataset $\{(x_1 = [1, 0], y_1 = 1), (x_2 = [1, 0], y_2 = -1)\}$ and exponential (logistic) loss using gradient descent with constant learning rate. Figure 2(a)(c)(e)(g) show how different choices of learning rate $\eta$ change the dynamics of loss function with exponential and logistic loss.

**Example 4.** Consider optimizing $\mathcal{L}(w)$ using one hidden layer linear networks with dataset $\{(x_1 = [1, 1], y_1 = -1), (x_2 = [1, -1], y_2 = 1), (x_3 = [-1, -2], y_3 = 1) \text{ and } (x_4 = [-1, 1], y_4 = 1)\}$ and exponential (logistic) loss using gradient descent with constant learning rate. Figure 2(b)(d)(f)(h) show how different choices of learning rate $\eta$ change the dynamics of loss function with exponential and logistic loss.

As Figure 2 shows, in the catapult phase, the eigenvalue of NTK decreases to a lower value than its initial point, while it keeps unchanged when the learning rate is small, which is in the lazy phase. For mean squared loss, the lower value of neural tangent kernel means the flatter curvature when the training loss is low [27]. However, whether it is valid for exponential and logistic loss is still unknown. We show that for degenerate data the Hessian matrix is equivalent to the NTK at the ending of training through the following corollary.

**Corollary 1.** (Informal) Consider optimizing $\mathcal{L}(w)$ with one hidden layer linear network under assumption 3 and exponential (logistic) loss using gradient descent with constant learning rate. For any constant learning rate that can converge to the global minimal, the larger the learning rate, the flatter curvature the gradient descent will achieve at the end of training.

We show the flatter curvature can be achieved in the catapult phase through Example 3 and 4 using the code provided by [35] to measure Hessian, as shown in Figure 3. In the lazy phase, both curvature and eigenvalue of NTK are independent of the learning rate at end of training. However, in the catapult phase the curvature decreases to the value smaller than that in the lazy phase. In conclusion, the NTK and Hessian at the end of training have the similar behavior on non-separable data.
Finally, we compare our results for the catapult phase with the result with mean squared loss and show the summary in Table 1.

Table 1: A summary of the relationship between data separability and the catapult phase for different loss functions

| separability                        | linear separable | degenerate | non-separable |
|-------------------------------------|------------------|------------|---------------|
| exponential loss (this work)       | ✗                | ✓          | ✓             |
| logistic loss (this work)           | ✗                | ✓          | ✓             |
| mean squared loss ([27])           | ✓                | ✓          | ✓             |

5 Experiment

We now study how the performance of linear networks with logistic loss on real data with respect to different learning rate phase. There is a correlation between the flatness of a minimum measured by curvature of Hessian and generalization performance [22], and this correlation has been confirmed in the catapult phase with mean squared loss [27]. Whether the correlation still holds for logistic loss given the fact that only non-separable or degenerate data can contribute to the catapult phase. We answer this question empirically by performing experiments on MNIST and CIFAR-10 datasets. For both data we select two of the classes to form a binary classification problem.

As shown in Figure 4, we find that the highest test accuracy can be achieved is the catapult phase. In Figure 4(a)(b), we show the phenomenon that can used to mark the catapult phase, which means the catapult phase exists in the real application. However, it is worth noting that the top eigenvalue of NTK slowly rises after a certain step at the very beginning. To explain this phenomenon, we need to know how the whole data is made up. According to the theorem 2 in [19], the data can be uniquely partitioned into linearly separable part and non-separable part. Thus the slowing rising phenomenon is caused by the linearly separable part since the solution for this part is at infinity.

In Figure 4(c)(d), we measure the test performance regarding different learning rates in both the lazy phase and the catapult phase. Note that the size of test set is much more than that of training set. We adopt this kind of partition for the data because the test accuracy for regular partition on MNIST often reach 1. In Figure 4(c), we show that highest test accuracy is achieved in the catapult phase. However, the comparison across different learning rate is not fair since the large learning rate runs faster naturally. To ensure a fair comparison, we use a fixed physical time which is defined as...
Figure 4: Training dynamics of gradient descent and test performance on MNIST dataset consists of number six and number nine with respect to different rate phase. One hidden layer linear network trained on MNIST with $\sigma_n^2 = 0.5$ and $m = 200$, the data size is $n_{\text{train}} = 50$ and $n_{\text{test}} = 6250$. (a)(b) Training loss as a function of time step $t$. (a) For the large learning rate, the loss grows at the beginning and then drop a low value while the loss keep decreasing at small learning rate. (b) Top eigenvalue of NTK denoted as $\lambda_0$ as a function of time step $t$. At the beginning, those with large learning rate increase and then drop to a lower value than their initial position, while NTK with small learning rate keep unchanged. After a certain step around $t = 3$, all NTK slowly rising. (c)(d) The generalization performance with respect to different learning rate. (c) The test accuracy is measured at the time step $t = 500$ for all learning rate. The best performance is in the catapult phase. (d) The test accuracy is measured at the time step $t = 500/\eta$ for corresponding learning rate. The best performance is in the catapult phase as well.

Figure 5: Test performance on CIFAR-10 dataset consists of cars and dogs with respect to different rate phase. The data size is $n_{\text{train}} = 2048$ and $n_{\text{test}} = 512$. (a)(b) We use a two-layer linear network without bias with $\sigma_n^2 = 0.5$ and $m = 500$. (a) The test accuracy is measured at the time step $t = 500$. (b) The test accuracy is measured at the physical time step $t = 50/\eta$ for no decay. Case while we use $t = 500$ more steps to train the network at $\eta = 0.01$ for decay case. (c)(d) We use a three-layer linear network with $\sigma_n^2 = 0.5$, $\sigma_n^2 = 0.01$, and $m = 500$. (c) The test accuracy is measured at the time step $t = 300$. (d) The test accuracy is measured at the physical time step $t = 50/\eta$ for no decay case while we use $t = 500$ more steps to train the network at $\eta = 0.01$ for decay case.

$t_{\text{ph}} = \eta t$. In this setting, the best performance is found in the catapult phase as well, which implies that the flatter minimum has a potential to generalize better in the real application.

Figure 5 shows the performance of two linear networks, one is one hidden layer without bias, and the other is two hidden layer linear network with bias, trained on CIFAR-10. If we fix the time step for all learning rates, the large learning rate has the advantage to obtain a certain test accuracy faster, as shown in Figure 5(a)(c). When we use a fixed physical time to conduct a fair comparison, the catapult phase does not show its potential to generalize better. However, to demonstrate the real power of flatter minimum, we adopt a learning decay scheme that training the network with more steps at a small learning rate after training at the original learning rate with physical time steps. Figure 5(b)(d) show that the best generalization performance is still happened in the catapult phase after adopting the learning decay scheme.

The result that the best generalization performance can be found in the catapult phase only occurs when we adopt the learning rate decay scheme for CIFAR-10 is consistent with what Yuanzhi Li et al. found as shown in [28]. The key insight in their analysis is that the order of learning different types of patterns is crucial: because the small learning rate model first memorizes easy-to-generalize, hard-to-fit patterns, it generalizes worse on hard-to-generalize, easier-to-fit patterns than its large
learning rate counterpart. In our work, the two patterns corresponding to linearly separable data and no-separable part. The large learning rate first achieves a flatter minimum for the non-separable data and then annealing to a small learning rate which can achieve implicit bias of maximum margin for the linearly separable part and has the advantage to generalize better [40]. In this sense, we name the influence of the large learning rate for non-separable data as the implicit bias.

6 Discussion

In this work, we show that the catapult phase exists with logistic loss because of the non (linearly)-separability. According to the theoretical analysis, loss in the catapult phase can converge to the global minimum as it in the lazy phase do, but a fatter minimum from the view of Hessian. Even without using SGD optimization, the optimal generalization performance can be achieve in the catapult phase with the help of learning rate decay scheme. Combined with the same results of mean squared loss case [27], our finding can be use to fill the gap between between the lazy training and real power of deep learning. In conclusion, we find that the implicit bias of deep linear networks in the large learning rate phase is realized by achieving a flatter global minimum. Finally, it is worth to study the role of large learning rate for nonlinear networks with (S)GD optimization and logistic loss, and we leave this open question for future work.

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A Appendix

This appendix is dedicated to proving the key results of this paper, namely Proposition 1 and Theorems 1, 2, and Corollary 1 which describe the dynamics of gradient descent with logistic and exponential loss in different learning rate phase.

Proposition 1. For a linear predictor $f = w^T x$, along with a loss $\ell \in \{\ell_{\text{exp}}, \ell_{\text{log}}\}$.

1. Under Assumption 1, the empirical loss is $\beta$-smooth. Then the gradient descent with constant learning rate $\eta < \frac{2}{\beta}$ never increase the risk, and empirical loss will converge to zero:

$$ \mathcal{L}(w(t+1)) - \mathcal{L}(w(t)) \leq 0, \quad \lim_{t \to \infty} \mathcal{L}(w(t)) = 0, \quad \text{with } \eta < \frac{2}{\beta} $$
2 Under Assumption 2, the empirical loss is $\beta$-smooth and $\alpha$-strongly convex, where $\alpha \leq \beta$. Then the gradient descent with a constant learning rate $\eta < \frac{2}{\beta}$ never increases the risk, and empirical loss will converge to a global minimum. On the other hand, the gradient descent with a constant learning rate $\eta > \frac{2}{\alpha}$ never decrease the risk, and empirical loss will explode or saturate:

$$ L(w(t + 1)) - L(w(t)) \leq 0, \quad \lim_{t \to \infty} L(w(t)) = G_0, \quad \text{with} \quad \eta < \frac{2}{\beta} $$

$$ L(w(t + 1)) - L(w(t)) \geq 0, \quad \lim_{t \to \infty} L(w(t)) = G_1, \quad \text{with} \quad \eta > \frac{2}{\alpha} $$

where $G_0$ is the value of global minimum while $G_1 = \infty$ for exploding situation or $G_0 < G_1 < \infty$ when saturating.

Proof. 1 We first prove that empirical loss $L(u)$ regrading data-scaled weight $u_i \equiv w^T x_i y_i$ for the linearly separable dataset is smooth. The empirical loss can be written as $L = \sum_{i=1}^{n} \ell(u_i)$, then the second derivatives of logistic and exponential loss are,

$$ L''_{\exp} = \sum_{i=1}^{n} \ell''_{\exp}(u_i) = \sum_{i=1}^{n} \exp''(-u_i) = \sum_{i=1}^{n} \exp(-u_i) $$

$$ L''_{\log} = \sum_{i=1}^{n} \ell''_{\log}(u_i) = \sum_{i=1}^{n} \log''(1 + \exp(-u_i)) = \sum_{i=1}^{n} \frac{\exp(-u_i)}{(1 + \exp(-u_i))^2} $$

when $w_i$ is limited, there will be a $\beta$ such that $L'' < \beta$. Besides, because there exists a separator $w_*$ such that $\forall i : w_*^T x_i y_i > 0$, the second derivative of empirical loss can be arbitrarily close to zero. This implies that the empirical loss function is not strongly convex.

Recall a property of $\beta$-smooth function $f$ [5].

$$ f(y) \leq f(x) + (\nabla_x f)^T (y - x) + \frac{1}{2} \beta \|y - x\|^2 $$

Taking the gradient descent into consideration,

$$ L(w(t + 1)) \leq L(w(t)) + (\nabla_{w(t)} L(w(t)))^T (w(t + 1) - w(t)) + \frac{1}{2} \beta \|w(t + 1) - w(t)\|^2 $$

$$ = L(w(t)) + (\nabla_{w(t)} L(w(t)))^T (w(t + 1) - w(t)) + \frac{1}{2} \beta \|w(t) - w(t)\|^2 $$

$$ = L(w(t)) - \eta(1 - \frac{\eta \beta}{2}) \|\nabla_{w(t)} L\|^2 $$

when $1 - \frac{\eta \beta}{2} > 0$, that is $\eta < \frac{2}{\beta}$, we have,

$$ L(w(t + 1)) \leq L(w(t)) - \eta(1 - \frac{\eta \beta}{2}) \|\nabla_{w(t)} L\|^2 \leq L(w(t)) $$

We now prove that empirical loss will converge to zero with learning rate $\eta < \frac{2}{\beta}$. We change the form of inequality above,

$$ \frac{L(w(t)) - L(w(t + 1))}{\eta(1 - \frac{\eta \beta}{2})} \geq \|\nabla_{w(t)} L(w(t))\|^2 $$

this implies,

$$ \sum_{t=0}^{T} \|\nabla_{w(t)} L(w(t))\|^2 \leq \sum_{t=0}^{T} \frac{L(w(t)) - L(w(t + 1))}{\eta(1 - \frac{\eta \beta}{2})} $$

$$ = \frac{L(w(0)) - L(w(T))}{\eta(1 - \frac{\eta \beta}{2})} < \infty $$

therefore we have $\lim_{t \to \infty} \|\nabla_{w(t)} L(w(t))\| = 0$. 

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2 When the data is not linear separable, there is no \( w_* \) such that \( \forall i : w_*^T x_i y_i > 0 \). Thus, at least one \( w_*^T x_i y_i \) is negative when the other terms are positive. This implies that the solution of the loss function is finite and the empirical loss is both \( \alpha \)-strongly convex and \( \beta \)-smooth.

Recall a property of \( \alpha \)-strongly convex function \( f \) [5],

\[
f(y) \geq f(x) + (\nabla_x f)^T (y - x) + \frac{1}{2\alpha} \|y - x\|^2
\]

Taking the gradient descent into consideration,

\[
\mathcal{L}(w(t + 1)) \geq \mathcal{L}(w(t)) + (\nabla_w \mathcal{L}(w(t)))^T (w(t + 1) - w(t)) + \frac{1}{2\alpha} \|w(t + 1) - w(t)\|^2
\]

\[
= \mathcal{L}(w(t)) + (\nabla_w \mathcal{L}(w(t)))^T (-\eta \nabla_w \mathcal{L}(w(t))) + \frac{1}{2\alpha} \|\nabla_w \mathcal{L}(w(t))\|^2
\]

\[
= \mathcal{L}(w(t)) - \eta (1 - \frac{\eta\alpha}{2}) \|\nabla_w \mathcal{L}(w(t))\|^2
\]

when \( 1 - \frac{\eta\alpha}{2} < 0 \), that is \( \eta > \frac{2}{\alpha} \), we have,

\[
\mathcal{L}(w(t + 1)) \geq \mathcal{L}(w(t)) - \eta (1 - \frac{\eta\alpha}{2}) \|\nabla_w \mathcal{L}(w(t))\|^2 \geq \mathcal{L}(w(t)).
\]

\( \square \)

**Theorem 1.** For a linear predictor \( f = w^T x \) equipped with exponential (logistic) loss under assumption 2 there is a critical learning rate that separates the whole learning rate space into two (three) regions, which is depends on the initial weight. The critical learning rate satisfies

\[
\mathcal{L}'(w(0)) = -\mathcal{L}'(w_0) - \eta_{\text{critical}} \mathcal{L}'(w(0)),
\]

where \( w(0) \) is the initial weight. Moreover,

1. For exponential loss, the gradient descent process with a constant learning rate \( \eta < \eta_{\text{critical}} \) never increases loss, and the empirical loss will converge to the global minimum. On the other hand, the gradient descent process with learning rate \( \eta = \eta_{\text{critical}} \) will oscillate. Finally, when the learning rate \( \eta > \eta_{\text{critical}} \), the training process never decreases the loss and the empirical loss will explode to infinity:

\[
\mathcal{L}(w(t + 1)) - \mathcal{L}(w(t)) < 0, \quad \lim_{t \to \infty} \mathcal{L}(w(t)) = 1, \quad \text{with} \quad \eta < \eta_{\text{critical}},
\]

\[
\mathcal{L}(w(t + 1)) - \mathcal{L}(w(t)) = 0, \quad \lim_{t \to \infty} \mathcal{L}(w(t)) = \mathcal{L}(w(0)), \quad \text{with} \quad \eta = \eta_{\text{critical}},
\]

\[
\mathcal{L}(w(t + 1)) - \mathcal{L}(w(t)) > 0, \quad \lim_{t \to \infty} \mathcal{L}(w(t)) = \infty, \quad \text{with} \quad \eta > \eta_{\text{critical}}.
\]

2. For logistic loss, the critical learning rate \( \eta_{\text{critical}} > 8 \). The gradient descent process with a constant learning rate \( \eta < 8 \) never increases the loss and the empirical loss will converge to the global minimum. On the other hand, the loss along the gradient descent process with a learning rate \( 8 \leq \eta < \eta_{\text{critical}} \) will not converge to global minimum but oscillate. Finally, when the learning rate \( \eta > \eta_{\text{critical}} \), it never decrease the distance the loss, and empirical loss will saturate:

\[
\mathcal{L}(w(t + 1)) - \mathcal{L}(w(t)) < 0, \quad \lim_{t \to \infty} \mathcal{L}(w(t)) = \log(2), \quad \text{with} \quad \eta < 8,
\]

\[
\mathcal{L}(w(t + 1)) - \mathcal{L}(w(t)) \leq 0, \quad \lim_{t \to \infty} \mathcal{L}(w(t)) = \mathcal{L}(w_*) < \mathcal{L}(w(0)), \quad \text{with} \quad 8 \leq \eta < \eta_{\text{critical}},
\]

\[
\mathcal{L}(w(t + 1)) - \mathcal{L}(w(t)) \geq 0, \quad \lim_{t \to \infty} \mathcal{L}(w(t)) = \mathcal{L}(w_*) \geq \mathcal{L}(w(0)), \quad \text{with} \quad \eta \geq \eta_{\text{critical}},
\]

where \( w_* \) satisfies \( -w_* = w_* - \frac{\eta \sinh(w_*)}{2(1 + \cosh(w_*)} \).

**Proof.**

1. Under the degeneracy assumption, the risk is given by the hyperbolic function \( \mathcal{L}(w_t) = \cosh(w_t) \). The update function for the single weight is,

\[
w_{k+1} = w_k - \eta \sinh(w_t).
\]
To compare the norm of the gradient $\|\sinh(w_t)\|$ and the norm of loss, we introduce the following function:

$$\phi(x) = \eta L'(x) - 2x = \eta \sinh(x) - 2x, \text{ for } x \geq 0.$$  \hfill (9)

Then it’s easy to see that

$$\mathcal{L}(w_{t+1}) > |\mathcal{L}(w_t)| \iff \phi(|w_t|) > 0.$$  

In this way, we have transformed the problem into studying the iso-surface of $\phi(x)$. Define Phase$_1$ by

$$\text{Phase}_1 = \{x|\phi(x) < 0\}.$$  

Let Phase$_2$ be the complementary set of Phase$_1$ in $[0, +\infty)$. Since $\frac{\sin x}{x}$ is monotonically increasing, we know that Phase$_2$ is connected and contains $+\infty$.

Suppose $\eta > \eta_{\text{critical}}$, then $\phi(w_0) > 0$, which implies that

$$\mathcal{L}(w_1) > \mathcal{L}(w_0) \text{ and } |w_1| > |w_0|.$$  

Thus, the first step gets trapped in Phase$_2$:

$$\phi(w_1) > 0.$$  

By induction, we can prove that $\phi(w_t) > 0$ for arbitrary $t \in \mathbb{N}$, which is equivalent to

$$\mathcal{L}(w_t) > \mathcal{L}(w_{t-1}).$$  

Similarly, we can prove the theorem under another toe initial conditions: $\eta = \eta_{\text{critical}}$ and $\eta < \eta_{\text{critical}}$.

2 Under the degeneracy assumption, the risk is governed by the hyperbolic function $\mathcal{L}(w_t) = \frac{1}{\pi} \log(2 + 2 \cosh(w_t))$. The update function for the single weight is,

$$w_{t+1} = w_t - \eta \frac{\sinh(w_t)}{2 1 + \cosh(w_t)}.$$  

Thus,

$$\phi(x) = \eta L'(x) - 2x = \eta \frac{\sinh(x)}{2 1 + \cosh(x)} - 2x, \text{ for } x \geq 0.$$  \hfill (11)

Unlike the exponential loss, $\frac{\sinh(x)}{2 1 + \cosh(x)}$ is monotonically decreasing, which means that Phase$_2$ of $\phi(x)$ doesn’t contain $+\infty$. (see figure 6).
Figure 7: Different colors represent different $\lambda$(NTK) values. (a) graph of $\phi_{\lambda}(x)$ equipped with the exponential loss. (b) graph of the derivative of $\phi_{\lambda}(x)$ equipped with the exponential loss. (c) graph of $\phi_{\lambda}(x)$ equipped with the logistic loss. (d) graph of the derivative of $\phi_{\lambda}(x)$ equipped with the logistic loss. Notice that the critical point of the exponential loss moves to the right as $\lambda$ decreases.

Suppose $8 < \eta < \eta_{\text{critical}}$, then $w_0$ lies in Phase 2. In this situation, we denote the critical point that separates Phase 1 and Phase 2 by $w_*$. That is

$$-w_* = w_0 - \eta \frac{\sinh(w_*)}{1 + \cosh(w_*)}.$$  

Then it’s obvious that before $w_t$ arrives at $w_*$, it keeps decreasing and will eventually get trapped at $w_*:

$$\lim_{t \to \infty} w_t = w_*,$$

and we have

$$\lim_{t \to \infty} \mathcal{L}(w_t) - \mathcal{L}(w_{t-1}) = 0.$$  

When $\eta < 8$, Phase 2 is empty. In this case, we can prove by induction that $\phi(w_t) > 0$ for arbitrary $t \in \mathbb{N}$, which is equivalent to

$$\mathcal{L}(w_t) > \mathcal{L}(w_{t-1}).$$

\[\square\]

**Theorem 2.** Under appropriate initialization and assumption 3, there exists a catapult phase for both the exponential and logistic loss. More precisely, when $\eta$ belongs to this phase, the output function $f(t)$ and the eigenvalue of NTK $\lambda(t)$ update in the following way:

1. $\mathcal{L}(t)$ keeps increasing when $t < T$.

2. After the $T$ step and its successors, the loss decreases, which is equivalent to:

$$|f(T+1)| > |f(T+2)| \geq |f(T+3)| \geq \ldots.$$  

3. The eigenvalue of NTK keeps dropping after the $T$ steps:

$$\lambda(T+1) > \lambda(T+2) \geq \lambda(T+3) \geq \ldots.$$  

Moreover, we have the inverse relation between the learning rate and the final eigenvalue of NTK:

$$\lambda(\infty) \leq \lim_{t \to \infty} \frac{4f(t)}{\eta_{\text{exp}}(t)} \text{ with exponential loss, or } \lambda(\infty) \leq \lim_{t \to \infty} \frac{4f(t)}{\eta_{\text{log}}(t)} \text{ with logistic loss.}$$
Proof. Exponential loss

\( \tilde{f}_{\exp} \) satisfies:

1. \( |\tilde{f}_{\exp}(x)| = |\tilde{f}_{\exp}(-x)| \).
2. \( \lim_{x \to 0} \frac{\tilde{f}_{\exp}(x)}{x} = 1 \).
3. \( \tilde{f}_{\exp}(x) \) has exponential growth as \( x \to \infty \).

By the definition of the normalized NTK, we automatically get

\[ \lambda(t) \geq 0. \]

From the numerical experiment, we observe that at the ending phase of training, \( \lambda(t) \) keeps non-increasing. Thus, \( \lambda(t) \) must converge to a non-negative value, which satisfies

\[ \frac{\eta^2}{m} \lambda^2 \tilde{f}_{\exp}(t) - \frac{4\eta}{m} f(t) \tilde{f}_{\exp}(t) \leq 0. \]  

(13)

Thus, \( \lambda \leq \lim_{t \to \infty} \frac{4f(t)}{\eta \tilde{f}_{\exp}(t)} \).

Since the output \( f \) converges to the global minimum, a larger learning rate will lead to a lower limiting value of the NTK. As it was pointed out in [27], a flatter NTK corresponds to a smaller generalization error in the experiment. However, we still need to verify that large learning rate exists.

Note that during training, the loss function curve may experience more than one wave of uphill and downhill. To give a precise definition of large learning rate, it should satisfy the following two conditions:

1. \( |f(T + 1)| > |f(T)| \), this implies that \( \mathcal{L}(T + 1) > \mathcal{L}(T) \).

For the \( T + 1 \) step and its successors,

\[ |f(T + 1)| > |f(T + 2)| \geq |f(T + 3)| \geq \ldots. \]

2. The norm of NTK keeps dropping after \( T \) steps:

\[ \lambda(T) > \lambda(T + 1) \geq \lambda(T + 2) \geq \ldots. \]

If we already know that the loss keeps decreasing after the \( T + 1 \) step, then

\[ \Delta \lambda = \frac{\eta}{m} \tilde{f} \cdot (\eta \lambda \tilde{f} - 4f). \]  

(14)

Since \( |\tilde{f}| \geq 1 \) and is monotonically increasing when \( \tilde{f} = \sinh f \), we automatically have

\[ \lambda_{\exp}(T) > \lambda_{\exp}(T + 1) > \lambda_{\exp}(T + 2) \geq \ldots, \]

If

\[ \lambda(T) < \frac{4f(T)}{\eta \tilde{f}(T)} \quad \text{and} \quad \lambda(T + 1) < \frac{4f(T + 1)}{\eta \tilde{f}(T + 1)}. \]

This condition holds if the parameters are close to zero initially.

To check condition (1), the following function which plays an essential role as in the non-hidden layer case:

\[ \phi_\lambda(x) = \eta \lambda \sinh(x) - \frac{\eta^2}{m} x \sinh^2(x) - 2x, \quad \text{for} \ x \geq 0. \]

Notice that an extra parameter \( \lambda \) emerges with the appearance of the hidden layer. We call it the control parameter of the function \( \phi(x) \).
For a fixed $\lambda$, since now $\phi(x)$ becomes linear, the whole $[0, +\infty)$ is divided into three phases (see Figure 7):

Phase$_1 := \{x \mid \phi_\lambda(x) < 0\}$ that contains 0,

Phase$_2 := \{x \mid \phi_\lambda(x) > 0\}$,

Phase$_3 := \{x \mid \phi_\lambda(x) < 0\}$ that contains $+\infty$.

It’s easy to see that $\mathcal{L}_\text{exp}(f(T + 1)) > \mathcal{L}_\text{exp}(f(T))$ if and only if

$$\phi_\lambda(T)(f(T)) > 0.$$  

That is, $f(T)$ lies in Phase$_2$ of $\phi_\lambda(T)$. Similarly,

$$\mathcal{L}_\text{exp}(f(T + 2)) < \mathcal{L}_\text{exp}(f(T + 1)) \iff \phi_\lambda(T + 1)(f(T + 1)) < 0.$$  

That is, $f(T + 1)$ jumps into Phase$_1$ of $\phi_\lambda(T + 1)$. Denote the point that separates Phase$_1$ and Phase$_2$ by $x_*$, then form the graph of $\phi_\lambda(x)$ with different $\lambda$, we know that

$$x_*(\lambda) > x_*(\lambda) \text{ if } \lambda' < \lambda.$$  

Therefore, condition (1) is satisfied if

$$x_*(\lambda(T + 1)) > f(T) + \phi_\lambda(T)(f(T)) \quad (15)$$  

and at the same time,

$$\lambda(T + 1) - \lambda(T) > 0.$$  

For simplicity, we reset $T$ as our initial step. Write the output function $f(t)$ as

$$f(t + 1) = f(t)(1 + A(t)), \quad (16)$$

where $A(t) = \frac{\eta^2}{m} \tilde{f}^2(t) - \eta \lambda(t) \tilde{f}(t)/t$. Thus, $\phi_\lambda(0)(f(0)) > 0$ is equivalent to $A(0) < -2$.

Similarly, write the update function for $\lambda(t)$ as

$$\lambda(t + 1) = \lambda(t)(1 + B(t)), \quad (17)$$

where $B(t) = \frac{\eta^2}{m} \tilde{f}^2(t) - \frac{4\eta}{m} \tilde{f}(t) f(t)/\lambda(t)$. To fulfill the above condition on NTK, we need

$$B(0) < 0.$$  

To check (15), let the initial output $f(0)$ be close to $X_*(\lambda_0)$ (this can be done by adjusting $w(0)$):

$$0 < f(0) - X_* < \epsilon.$$  

Then by the mean value theorem,

$$x_*(\lambda(1)) - x_*(\lambda(0)) = \frac{\partial x_*}{\partial \lambda_*}(\lambda_0) \cdot \Delta \lambda.$$  

The derivative $\frac{\partial x_*}{\partial \lambda_*}$ can be calculated by the implicit function theorem:

$$\frac{\partial x_*}{\partial \lambda} = -\frac{\partial \phi_\lambda(x_*)}{\partial \lambda} \cdot \frac{\partial \phi_\lambda(x_*)}{\partial x_*}$$  

$$= -\eta \sinh(x_*) \cdot \frac{\partial \phi_\lambda(x_*)}{\partial x_*}.$$  

It’s easy to see that $|\frac{\partial x_*}{\partial \lambda_*}|$ is bounded away from zero if the initial output is in Phase$_2$ and near $x_*$ of $\phi_\lambda(0)(x)$ (see Figure 7).

On the other hand, we have the freedom to move $f(0)$ towards $x_*$ of $\phi_\lambda(0)(x)$ without breaking the $\Delta \lambda < 0$ condition. Since

$$|\frac{\eta \lambda_0 \tilde{f}}{4f}| < |\frac{\eta \lambda_0 \tilde{f}'}{4f'}| \quad \text{if } f < f'.$$  

Therefore, we can always find a $\epsilon > 0$ such that $0 < f(0) - x_* < \epsilon$ and (15) is satisfied. Combining the above, we have demonstrated the existence of the \textit{catapult phase} for the exponential loss.
logistic loss

When Considering the degeneracy case for the logistic loss, the loss will be
\[
\mathcal{L} = \frac{1}{2} \log(2 + 2 \cosh(m^{-1/2} w^{(2)}(w^{(1)}))).
\] (18)

Much of the argument is similar. For example, Equation (13) still holds if we replace \( \tilde{f}_{\text{exp}} \) by
\[
\tilde{f}_{\log}(x) := \frac{\sinh(x)}{1 + \cosh(x)}.
\]

\( \tilde{f}_{\log} \) satisfies
1. \( |\tilde{f}_{\log}(x)| = |\tilde{f}_{\log}(-x)| \).
2. \( |\tilde{f}_{\log}(x)| \leq 1 \) for \( x \in (-\infty, \infty) \).

This implies that \( |\tilde{f}| \leq \frac{1}{2} \).

Then by (14), we have \( \Delta \lambda < 0 \) if \( \lambda \leq \frac{8}{\eta} \). Thus, condition 2 is satisfied for both loss functions. Now, \( \phi_{\lambda}(x) \) becomes:
\[
\phi_{\lambda}(x) := \eta \lambda \frac{\sinh(x)}{1 + \cosh(x)} - \frac{\eta^2 m}{2} \sinh^2(x) (1 + \cosh(x))^2 - 2x,
\]
along with its derivative:
\[
\phi'_{\lambda}(x) := \eta \lambda \frac{\cosh(x)}{1 + \cosh(x)} - \frac{\eta^2 m}{2} \sinh^2(x) (1 + \cosh(x))^2 - 2x - \frac{\eta^2}{m} \sinh(x) \left[ \frac{\cosh(x)}{1 + \cosh(x)} - \frac{\sinh^2(x)}{(1 + \cosh(x))^2} \right].
\]

The method of verifying condition 1 is similar with the exponential case, except that \( \phi_{\lambda}(x) \) has only Phase\(_1\) and Phase\(_2\) (see figure[7]). As the NTK \( \lambda \) goes down, Phase\(_2\) will disappear and at that moment the loss will keep decreasing. Let \( \lambda_* \) be the value such that \( \phi'_{\lambda_*}(x) = 0 \), then
\[
\lambda_* = 4/\eta.
\]

During the period when \( 4/\eta < \lambda_t < 8/\eta \), the NTK keeps dropping and the loss may oscillate around \( x_* \). However, we may encounter the scenario that both the loss and the \( \lambda_t \) are going up before dropping down simultaneously (see the first three steps in figure[7]). Theoretically, it corresponds to jump from Phase\(_2\) to Phase\(_3\) and then to Phase\(_1\) of \( \phi_{\lambda}(x) \) in the first two steps. This is possible since \( \tilde{f}_{\log} \) is decreasing when \( x > 0 \). This implies that
\[
\frac{|\eta \lambda \tilde{f}'}{4f'} < \frac{|\eta \lambda \tilde{f}|}{4f} \text{ if } f < f'.
\]

So an increase of the output will cause the NTK to drop faster.

**Corollary 1. (Informal)** Consider optimizing \( \mathcal{L}(w) \) with one hidden layer linear network under assumption[6] and exponential (logistic) loss using gradient descent with constant learning rate. For any constant learning rate that can converge to the global minimal, the larger the learning rate, the flatter curvature the gradient descent will achieve at the end of training.

**Proof.** The Hessian matrix is defined as the second derivatives of the loss with respect to the parameters,
\[
H_{\alpha\beta} = \frac{\partial^2 \mathcal{L}}{\partial \theta_\alpha \partial \theta_\beta}.
\]
where $\theta_\alpha, \theta_\beta \in \{w^{(1)}, w^{(2)}\}$ for our setting of linear networks. For logistic loss,

$$H_{\alpha\beta} = \frac{1}{n} \sum_i \frac{\partial^2 \exp(-y_i f_i)}{\partial \theta_\alpha \partial \theta_\beta}$$

$$= \frac{1}{n} \sum_i \left[ \frac{\partial^2 f_i}{\partial \theta_\alpha \partial \theta_\beta} \exp(-y_i f_i)(y_i) + \frac{\partial f_i}{\partial \theta_\alpha} \frac{\partial f_i}{\partial \theta_\beta} \exp(-y_i f_i) \right]$$

We want to make a connection from Hessian matrix to the neural tangent kernel. Note that the second term contains $\frac{\partial f_i}{\partial \theta_\alpha}, \frac{\partial f_i}{\partial \theta_\beta}$, which can be written as $JJ^T$, where $J = \text{vec} \frac{\partial f_i}{\partial \theta}$, While NTK can be expressed as $JJ^T J$. It is known that they have the same eigenvalue. Further more, under assumption 3 we have $n = 2$ and $f_1 = f_2$, thus,

$$H_{\alpha\beta} = \frac{1}{n} \sum_i \left[ \frac{\partial^2 f_i}{\partial \theta_\alpha \partial \theta_\beta} \frac{\partial L}{\partial f_0} + \frac{\partial f_i}{\partial \theta_\alpha} \frac{\partial f_i}{\partial \theta_\beta} \frac{\partial L}{\partial f_0} \right]$$

Suppose at the end of gradient descent training, we can achieve global minimal. Then we have, $\frac{\partial L}{\partial f_0} = 0$, and $L = 1$. Thus, the Hessian matrix reduce to,

$$H_{\alpha\beta} = \frac{1}{n} \sum_i \frac{\partial f_i}{\partial \theta_\alpha} \frac{\partial f_i}{\partial \theta_\beta}$$

In this case, the eigenvalues of Hessian matrix are equal to those of neural tangent kernel. Combine with the[2] we can prove the result.

For logistic loss,

$$H_{\alpha\beta} = \frac{1}{n} \sum_i \frac{\partial^2 \log(1 + \exp(-y_i f_i))}{\partial \theta_\alpha \partial \theta_\beta}$$

$$= \frac{1}{n} \sum_i \left[ \frac{\partial^2 f_i}{\partial \theta_\alpha \partial \theta_\beta} \exp(-y_i f_i)(y_i) + \frac{\partial f_i}{\partial \theta_\alpha} \frac{\partial f_i}{\partial \theta_\beta} \frac{\exp(-y_i f_i)}{1 + \exp(-y_i f_i)} \exp(-y_i f_i) \right]$$

Under assumption 3 we have $n = 2$ and $f_1 = f_2$, thus,

$$H_{\alpha\beta} = \frac{1}{n} \sum_i \left[ \frac{\partial^2 f_i}{\partial \theta_\alpha \partial \theta_\beta} \frac{\partial L}{\partial f_0} + \frac{\partial f_i}{\partial \theta_\alpha} \frac{\partial f_i}{\partial \theta_\beta} \frac{\exp(-y_i f_i)}{1 + \exp(-y_i f_i)} \right]$$

Suppose at the end of gradient descent training, we can achieve global minimal. Then we have, $\frac{\partial L}{\partial f_0} = 0$, and $f_i = 0$. Thus, the Hessian matrix reduce to,

$$H_{\alpha\beta} = \frac{1}{4n} \sum_i \frac{\partial f_i}{\partial \theta_\alpha} \frac{\partial f_i}{\partial \theta_\beta}$$

In this case, the eigenvalues of Hessian matrix and NTK have the relation $\frac{1}{2} \lambda_{\text{NTK}} = \lambda_{\text{Hessian}}$. 

\textbf{B} \quad \textbf{Supplementary material}

The update equations for the output and kernel evaluated on general training set with logistic loss are,

$$f_\alpha(t+1) = f_\alpha(t) - \eta \Theta_{\alpha\beta} \frac{\partial f_\alpha}{\partial f_0}(\zeta_j x_{ja})$$

$$\Theta_{\alpha\beta}(t+1) = \Theta_{\alpha\beta}(t) - \frac{\eta}{mn} \left[ f_\alpha(\zeta_j x_{ja}) + f_\beta(\zeta_j x_{ja}) + \frac{2}{n} (\bar{f}_\alpha f_\alpha)(x_{ja} x_{j\beta}) \right]$$

$$+ \frac{\eta^2}{2mn^2} \left[ (u_{ij}^2)^2 (\zeta_j x_{j\alpha})(\zeta_j x_{j\beta}) + (u_{i\alpha} \zeta_j)(u_{i\beta} \zeta_j)) (x_{ja} x_{j\beta}) \right],$$

where $\bar{f}_\alpha = \frac{y_{\alpha 0} e^{-y_0 f(x_{\alpha})}}{1 + e^{-y_0 f(x_{\alpha})}}$, and $\zeta_j = \frac{1}{n} \sum \bar{f}_\alpha x_{ja}$.