Optimization for deep learning: an overview

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Abstract

Optimization is a critical component in deep learning. We think optimization for neural networks is an interesting topic for theoretical research due to various reasons. First, its tractability despite non-convexity is an intriguing question, and may greatly expand our understanding of tractable problems. Second, classical optimization theory is far from enough to explain many phenomenons. Therefore, we would like to understand the challenges and opportunities from a theoretical perspective, and review the existing research in this field. First, we discuss the issue of gradient explosion/vanishing and the more general issue of undesirable spectrum, and then discuss practical solutions including careful initialization, normalization methods, and skip connections. Second, we review generic optimization methods used in training neural networks, such as stochastic gradient descent (SGD) and adaptive gradient methods, and existing theoretical results. Third, we review existing research on the global issues of neural network training, including results on global landscape, mode connectivity, lottery ticket hypothesis and neural tangent kernel (NTK).

1 Introduction

Optimization has been a critical component of neural network research for a long time. However, it is not clear at first sight whether neural network problems are good topics for theoretical study, as they are both too simple and too complicated. On one hand, they are "simple" because typical neural network problems are just a special instance of a unconstrained continuous optimization problem (this view is problematic though, as argued later), which is itself a subarea of optimization. On the other hand, neural network problems are indeed "complicated" because of the composition of many non-linear functions. If we want to open the "black box" of the neural networks and look carefully at the inner structure, we may find ourselves like a child in a big maze with little clue what is going on. In contrast to the rich theory of many optimization branches such as convex optimization and integer programming, the theoretical appeal of this special yet complicated unconstrained problem is not clear.

That being said, there are a few reasons that make neural network optimization an interesting topic of theoretical research. First, neural networks may provide us a new class of tractable op-

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timization problems beyond convex problems. A somewhat related analogy is the development of conic optimization: in 1990's, researchers realized that many seemingly non-convex problems can actually be reformulated as conic optimization problems (e.g. semi-definite programming) which are convex problems, thus the boundary of tractability has advanced significantly. Neural network problems are surely not the worst non-convex optimization problems and their global optima could be found relatively easily in many cases. Admittedly, they are also not the best non-convex problems either. In fact, they are like wild animals and proper tuning is needed to make them work, but if we can understand their behavior and tame these animals, they will be very powerful tools to us.

Second, existing nonlinear optimization theory is far from enough to explain the practical behavior of neural network training. A well known difficulty in training neural-nets is called "gradient explosion/vanishing" due to the concatenation of many layers. Properly chosen initialization and/or other techniques are needed to train deep neural networks, but not always enough. This poses a great challenge for theoretical analysis, because what conditions are needed for theoretical analysis is not very clear. Even proving convergence (to stationary points) of the existing method with the practically used stepsize seems a difficult task. In addition, some seemingly simple methods like SGD with cyclical step-size and Adam work very well in practice, and the current theory is far from explaining their effectiveness. Overall, there is still much space for rigorous convergence analysis and algorithm design.

Third, although the basic formulation a theoretician has in mind (and the focus of this article) is an unconstrained problem, neural network is essentially a way to parametrize the optimization variable and thus can be applied to a wide range of problems, including reinforcement learning and min-max optimization. In principle, any optimization problem can be combined with neural networks. As long as a cascade of multiple parameters appears, the problem suddenly faces all the issues we discussed above: the parametrization may cause complicated landscape, and the convergence analysis may be quite difficult. Understanding the basic unconstrained formulation is just the first step towards understanding neural networks in a broader setting, and presumably there can be richer optimization theory or algorithmic ingredients that can be developed.

To keep the survey simple, we will focus on the supervised learning problem with feedforward neural networks. We will not discuss more complicated formulations such as GANs (generative adversarial networks) and deep reinforcement learning, and do not discuss more complicated architecture such as RNN (recurrent neural network), attention and Capsule. In a broader context, theory for supervised learning contains at least representation, optimization and generalization (see Section 1.1), and we do not discuss representation and generalization in detail.

This article is written for researchers who are interested in theoretical understanding of optimization for neural networks. Prior knowledge on optimization methods and basic theory will be very helpful (see, e.g., [23, 189, 30] for preparation). Existing surveys on optimization for deep learning are intended for general machine learning audience, such as Chapter 8 of the book Goodfellow et al. [75]. These surveys often do not discuss optimization theoretical aspects in depth. In contrast, in this article, we emphasize more on the theoretical results while trying to make it accessible for non-theory readers. Simple examples that illustrate the intuition will be provided if possible, and we will not explain the details of the theorems.

1.1 Big picture: decomposition of theory

A useful and popular meta-method to develop theory is decomposition. We first briefly review the role of optimization in machine learning, and then discuss how to decompose the theory of optimization for deep learning.

Representation, optimization and generalization. The goal of supervised learning is to find a function that approximates the underlying function based on observed samples. The first step is to find a rich family of functions (such as neural networks) that can represent the desirable function. The second step is to identify the parameter of the function by minimizing a certain loss function. The third step is to use the function found in the second step to make predictions on unseen test data, and the resulting error is called test error. The test error can be decomposed into representation error, optimization error and generalization error, corresponding to the error caused by each of the three steps.

In machine learning, the three subjects representation, optimization and generalization are often studied separately. For instance, when studying representation power of a certain family of functions, we often do not care whether the optimization problem can be solved well. When studying the generalization error, we often assume that the global optima have been found (see [93] for a survey of generalization). Similarly, when studying optimization properties, we often do not explicitly consider the generalization error (but sometimes we assume the representation error is zero).

Decomposition of optimization issues. Optimization issues of deep learning are rather complicated, and further decomposition is needed. The development of optimization can be divided into three steps. The first step is to make the algorithm start running and converge to a reasonable solution such as a stationary point. The second step is to make the algorithm converge as fast as possible. The third step is to ensure the algorithm converge to a solution with a low objective value (e.g. global minima). There is an extra step of achieving good test accuracy, but this is beyond the scope of optimization. In short, we divide the optimization issues into three parts: convergence, convergence speed and global quality.

$$\text{Optimization issues} \begin{cases} \text{Local issues} \begin{cases} \text{Convergence issue: gradient explosion/vanishing} \\ \text{Convergence speed issue} \end{cases} \\ \text{Global issues: bad local minima, plaeaus, etc.} \end{cases}$$

Most works are reviewed in three sections: Section 4, Section 5 and Section 6. Roughly speaking, each section is mainly *motivated* by one of the three parts of optimization theory. However, this partition is not precise as the boundaries between the three parts are blurred. For instance, some techniques discussed in Section 4 can also improve the convergence rate, and some results in Section 6 address the convergence issue as well as global issues. Another reason of the partition is that

Optimization terms	optimization variable	objective	stepsize
Deep learning terms	weight, parameter	training loss	learning rate

Table 1: Optimization and machine learning terminology: the terms in the same column represent the same thing.

they represent three rather separate subareas of neural network optimization, and are developed somewhat independently.

1.2 Terminology and Outline

Terminology. The terminology of optimization and deep learning are somewhat different, and in this article we use them interchangeably. See Table 1 for a comparison of some major terms.

Outline. The structure of the article is as follows. In Section 2, we present the formulation of a typical neural network optimization problem for supervised learning. In Section 3, we present back propagation (BP) and discuss the basic convergence results. In Section 4, we discuss neural-net specific tricks for training a neural network, and some underlying theory. In particular, we discuss a major challenge called gradient explosion/vanishing, and review main solutions such as careful initialization and normalization methods. In Section 5, we discuss generic algorithm design which treats neural networks as generic non-convex optimization problems. In particular, we review SGD with various learning rate schedules, adaptive gradient methods, large-scale distributed training, second order methods and the existing convergence and iteration complexity results. In Section 6, we review research on global optimization of neural networks, including global landscape, mode connectivity, lottery ticket hypothesis and neural tangent kernel (NTK).

2 Problem Formulation

In this section, we present the optimization formulation for a supervised learning problem. Suppose we are given data points $x_i \in \mathbb{R}^{d_x}, y_i \in \mathbb{R}^{d_y}, i = 1, \dots, n$, where n is the number of samples. The input instance x_i can represent a feature vector of an object, an image, a vector that presents a word, etc. The output instance y_i can represent a real-valued vector or scalar such as in a regression problem, or an integer-valued vector or scalar such as in a classification problem.

We want the computer to predict y_i based on the information of x_i, so we want to learn the underlying mapping that maps each x_i to y_i. To approximate the mapping, we use a neural network $f_\theta : \mathbb{R}^{d_x} \to \mathbb{R}^{d_y}$, which maps an input x to a predicted output $\hat{y}$. A standard fully-connected neural network is given by

$$f_\theta(x) = W^L \phi(W^{L-1} \dots \phi(W^2 \phi(W^1 x))), \tag{1}$$

where $\phi : \mathbb{R} \to \mathbb{R}$ is the neuron activation function (sometimes simply called "activation" or "neuron"), W^j is a matrix of dimension $d_j \times d_{j-1}$, $j = 1, \dots, L$ and $\theta = (W^1, \dots, W^L)$ represents the collection of all parameters. Here we define $d_0 = d_x$ and $d_L = d_y$. When applying the scalar function ϕ to a vector v, we apply ϕ to each entry of v. Another way to write down the neural network is to use a recursion formula:

$$z^0 = x; \quad z^l = \phi(W^l z^{l-1}),\ l = 1, \ldots, L. \tag{2}$$

Note that in practice, the recursive expression should be $z^l = \phi(W^l z^{l-1} + b^l)$. For simplicity of presentation, throughout the paper, we often skip the "bias" term b^l in the expression of neural networks and just use the simplified version (2).

We want to pick the parameter of the neural network so that the predicted output $\hat{y}_i = f_\theta(x_i)$ is close to the true output y_i, thus we want to minimize the distance between y_i and $\hat{y}_i$. For a certain distance metric $\ell(\cdot, \cdot)$, the problem of finding the optimal parameters can be written as

$$\min_\theta F(\theta) \triangleq \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\theta(x_i)). \tag{3}$$

For regression problems, $\ell(y, z)$ is often chosen to be the quadratic loss function $\ell(y, z) = \|y - z\|^2$. For binary classification problem, a popular choice of ℓ is $\ell(y, z) = \log(1 + \exp(-yz))$.

Technically, the neural network given by (2) should be called fully connected feed-forward networks (FCN). Neural networks used in practice often have more complicated structure. For computer vision tasks, convolutional neural networks (CNN) are standard. In natural language processing, extra layers such as "attention" are commonly added. Nevertheless, for our purpose of understanding the optimization problem, we mainly discuss the FCN model (2) throughout this article, though in few cases the results for CNN will be mentioned.

For a better understanding of the problem (3), we relate it to several classical optimization problems.

2.1 Relation with Least Squares

One special form of (3) is the linear regression problem (least squares):

$$\min_{w \in \mathbb{R}^{d \times 1}} \|y - w^T X\|^2, \tag{4}$$

where $X = (x_1, \ldots, x_n) \in \mathbb{R}^{d \times n}$, $y \in \mathbb{R}^{1 \times n}$. If there is only one linear neuron that maps the input x to $w^T x$ and the loss function is quadratic, then the general neural network problem (3) reduces to the least square problem (4). We explicitly mention the least square problem for two reasons. First, it is one of the simplest forms of a neural network problem. Second, when understanding neural network optimization, researchers have constantly resorted to insight gained from analyzing linear regression.

2.2 Relation with Matrix Factorization

Neural network optimization (3) is closely related to a fundamental problem in numerical computation: matrix factorization. If there is only one hidden layer of linear neurons and the loss function is quadratic, and the input data matrix X is the identity matrix, the problem (3) reduces to

$$\min_{W_1, W_2} \|Y - W_2 W_1\|_F^2, \tag{5}$$

where $W_2 \in \mathbb{R}^{d_y \times d_1}$, $W_1 \in \mathbb{R}^{d_1 \times n}$, $Y \in \mathbb{R}^{d_y \times n}$ and $\|\cdot\|_F$ indicates the Frobenious norm of a matrix. If $d_1 < \min\{n, d_y\}$, then the above problem gives the best rank-d_1 approximation of the matrix Y. Matrix factorization is widely used in engineering, and it has many popular extensions such as non-negative matrix factorization and low-rank matrix completion. Neural network can be viewed as an extension of two-factor matrix factorization to multi-factor nonlinear matrix factorization.

3 Gradient Descent: Implementation and Basic Analysis

A large class of methods for neural network optimization are based on gradient descent (GD). The basic form of GD is

$$\theta_{t+1} = \theta_t - \eta_t \nabla F(\theta_t), \tag{6}$$

where η_t is the step-size (a.k.a. "learning rate") and $\nabla F(\theta_t)$ is the gradient of the loss function for the t-th iterate.

In the rest of the section, we first discuss the computation of the gradient by "backpropagation", then discuss classical convergence analysis for GD.

3.1 Computation of Gradient: Backpropagation

The discovery of backpropagation (BP) was considered an important landmark in the history of neural networks. From an optimization perspective, it is just an efficient implementation of gradient computation [1]. To illustrate how BP works, suppose the loss function is quadratic and consider the *per-sample* loss of the non-linear network problem $F_i(\theta) = \|y_i - W^L \phi(W^{L-1} \dots W^2 \phi(W^1 x_i))\|^2$. The derivation of BP applies to any i, thus for simplicity of presentation we ignore the subscript i, and use x and y instead. In addition, to distinguish the per-sample loss with the total loss $F(\theta)$, we use $F_0(\theta)$ to denote the per-sample loss function:

$$F_0(\theta) = \|y - W^L \phi(W^{L-1} \dots W^2 \phi(W^1 x))\|^2. \tag{7}$$

We define an important set of intermediate variables:

$$\begin{aligned} z^0 &= x, & h^1 &= W^1 z^0, \\ z^1 &= \phi(h^1), & h^2 &= W^2 z^1, \\ &\vdots, & &\vdots \\ z^{L-1} &= \phi(h^{L-1}), & h^L &= W^L z^{L-1}. \end{aligned} \tag{8}$$

[1] While using GD to solve an optimization problem is straightforward, discovering BP is historically nontrivial.

Here, h^l is often called pre-activation since it is the value that flows into the neuron, and z^l is called post-activation since it is the value comes out of the neuron. Further, define $D^l = \text{diag}(\phi'(h^l_1), \ldots, \phi'(h^l_{d_l}))$, which is a diagonal matrix with the t-th diagonal entry being the derivative of the activation function evaluated at the t-th pre-activation h^l_t.

Let the error vector $e = 2(h^L - y)$ [2]. The gradient over weight matrix W^l is given by

$$\frac{\partial F_0}{\partial W^l} = (W^L D^{L-1} \ldots W^{l+2} D^{l+1} W^{l+1} D^l)^T e (z^{l-1})^T, \quad l = 1, \ldots L. \tag{9}$$

Define a sequence of backpropagated error as

$$\begin{aligned} e^L &= e, \\ e^{L-1} &= (D^{L-1} W^L)^T e^L, \\ &\ldots, \\ e^1 &= (D^1 W^2)^T e^2. \end{aligned} \tag{10}$$

Then the partial gradient can be written as

$$\frac{\partial F_0}{\partial W^l} = e^l (z^{l-1})^T, \quad l = 1, 2, \ldots, L. \tag{11}$$

This expression does not specify the details of computation. A naive method to compute all partial gradients would require $O(L^2)$ matrix multiplications since each partial gradient requires $O(L)$ matrix multiplications. Many of these multiplication are repeated, thus a smarter algorithm is to reuse the multiplications, similar to the memorization trick in dynamical programming. More specifically, the algorithm back-propagation computes all partial gradients in a forward pass and a backward pass. In the forward pass, from the bottom layer 1 to the top layer L, post-activation z^l is computed recursively via (8) and stored for future use. After computing the last layer output $f_\theta(x) = h^L$, we compare it with the ground-truth y to obtain the error $e = \ell(h^L, y)$. In the backward pass, from the top layer L to the bottom layer 1, two quantities are computed at each layer l. First, the backpropagated error e^l is computed according to (10), i.e., left-multiplying e^{l+1} by the matrix $(D^{l-1} W^l)^T$. Second, the partial gradient over the l-th layer weight matrix W^l is computed by (11), i.e., multiply the backward signal e^l and the pre-stored feedforward signal $(z^{l-1})^T$. After the forward pass and the backward pass, we have computed the partial gradient for each weight (for one sample x). By a small modification to this procedure, we can implement stochastic gradient method instead of GD, which we skip here.

Rigorously speaking, the term "backpropagation" refers to algorithm that computes the partial gradients, i.e., for a mini-batch of samples, computing the partial gradients in one forward pass and one backward pass. Nevertheless, it is also often used to describe the entire learning algorithm, especially SGD.

[2] If the loss function is not quadratic, but a general loss function $\ell(y, h^L)$, we only need to replace $e = 2(h^L - y)$ by $e = \frac{\partial \ell}{\partial h^L}$.

3.2 Basic Convergence Analysis of GD

In this subsection, we discuss what classical convergence results can be applied to a neural network problem with minimal assumptions. Convergence analysis tailored for neural networks under strong assumptions will be discussed in Section 6. Consider the following question:

$$\text{Does gradient descent converge for neural network optimization (3)?} \tag{12}$$

Meaning of "convergence". There are multiple criteria of convergence. Although we wish that the iterates converge to a global minimum, a more common statement in classical results is "every limit point is a stationary point" (e.g. [23]). Besides the gap between stationary points and global minima (will be discussed in Section 6), this claim does not exclude a few undesirable cases: (U1) the sequence could have more than one limit points; (U2) limit points could be non-existent [3], i.e., the sequence of iterates can diverge. For this section, let us be satisfied with this criterion of convergence.

Convergence theorems. There are mainly two types of convergence results for gradient descent. Proposition 1.2.1 in [23] applies to the minimization of any differentiable function, but it requires line search that is relatively uncommon in large-scale training due to the computation cost, so we skip it here. A result more well-known in machine learning area requires Lipschitz smooth gradient. Proposition 1.2.3 in [23] states that if $\|\nabla F(w) - \nabla F(v)\| \leq \beta \|w - v\|$ for any w and v, and we use GD with constant stepsize less than $2/\beta$ to solve the problem, then every limit point of the sequence generated by this algorithm is a stationary point.

These theorems require the existence of a global Lipschitz constant β of the gradient. However, for neural network problem (3) a global Lipschitz constant does not exist, thus there is a gap between the theory and practice. Is there a simple way to fix this gap?

One solution is to add an assumption that the iterates are always bounded. Another simple solution is to add a ball constraint to the network parameters, and use gradient projection (GP) method. The gradient is Lipschitz continuous in a ball, then according to Proposition 2.3.2 of [23] every limit point of the sequence produced by GP with stepsize less than $2/\beta$ is a stationary point (which is not the point satisfying $\nabla F(w) = 0$ but the KKT point of the ball-constrained problem). Using a ball constraint is not theoretically perfect due to various reasons (e.g. many results discussed in this survey are proved for unconstrained problems, which do not directly apply to constrained problems), but can be a reasonable justification of gradient descent type methods. A bigger challenge is that the Lipschitz constant can be very large or small, causing a major training difficulty. This is closely related to "gradient explosion/vanishing", and the point of departure for the next section.

[3] In logic, the statement "every element of the set A belongs to the set B" does not imply the set A is non-empty; if the set A is empty, then the statement always holds. For example, "every dragon on the earth is green" is a correct statement, since no dragon exists.

4 Neural-net Specific Tricks

Without any prior experience, training a neural network to achieve a reasonable accuracy can be rather challenging. Nowadays, after decades of trial and research, people can train a large network relatively easily (at least for some applications such as image classification). In this section, we will describe some main tricks needed for training a neural network.

4.1 Possible Slow Convergence Due to Explosion/Vanishing

The most well-known difficulty of training deep neural-nets is probably gradient explosion/vanishing. A common description of gradient explosion/vanishing is from a signal processing perspective. Gradient descent can be viewed as a feedback correction mechanism: the error at the output layer will be propagated back to the previous layers so that the weights are adjusted to reduce the error. Intuitively, when signal propagates through multiple layers, it may get amplified at each layer and thus explode, or get attenuated at each layer and thus vanish. In both cases, the update of the weights will be problematic.

We illustrate the issue of gradient explosion/vanishing via a simple example of 1-dimensional problem:

$$\min_{w_1, w_2, \ldots, w_L \in \mathbb{R}} F(w) \triangleq 0.5(w_1 w_2 \ldots w_L - 1)^2. \tag{13}$$

The gradient over w_i is

$$\nabla_{w_i} F = w_1 \ldots w_{i-1} w_{i+1} \ldots w_L (w_1 w_2 \ldots w_L - 1) = w_1 \ldots w_{i-1} w_{i+1} \ldots w_L e, \tag{14}$$

where $e = w_1 w_2 \ldots, w_L - 1$ is the error. If all $w_j = 2$, then the gradient has norm $2^{L-1}|e|$ which is exponentially large; if all $w_j = 1/2$, then the gradient has norm $0.5^{L-1}e$ which is exponentially small.

Example: $F(w) = (w^7 - 1)^2$, where $w \in \mathbb{R}$ (similar to the example analyzed in [180]). This is a simpler version of (13). The plot of the function is provided in Figure 1. The region $[-1 + c, 1 - c]$ is flat, which corresponds to vanishing gradient (here c is a small constant, e.g. 0.2). The regions $[1 + c, \infty]$ and $[-\infty, -1 - c]$ are steep, which correspond to exploding gradient. Near the global minimum $w = 1$, there is a good basin that if initializing in this region GD can converge fast. If initializing outside this region, say, at $w = -1$, then the algorithm has to traverse the flat region with vanishing gradients which takes a long time. This is the main intuition behind [180] which proves that it takes exponential time (exponential in the number of layers L) for GD with constant stepsize to converge to a global minimum if initializing near $w_i = -1, \forall i$.

Theoretically speaking, why is gradient explosion/vanishing a challenge? This 1-dimensional example shows that gradient vanishing can make GD with constant stepsize converge very slowly. In general, the major drawback of gradient explosion/vanishing is the non-convergence within polynomial time, due to a large condition number of Hessian matrices and difficulty in picking a proper step-size. More specifically, gradient explosion/vanishing will affect the convergence speed

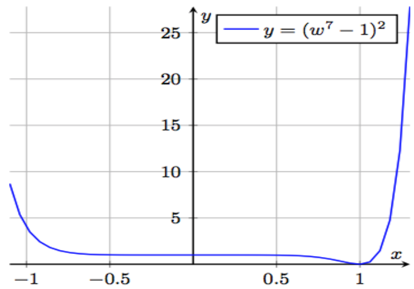


Figure 1: Plot of the function $F(w) = (w^7 - 1)^2$, which illustrates the gradient explosion/vanishing issues. In the region $[-0.8, 0.8]$, the gradients almost vanish; in the region $[1.2, \infty]$ and $[-\infty, -0.8]$, the gradients explode.

in the following way. First, the convergence speed is often determined by the condition number of the Hessian matrices. Gradient explosion/vanishing means that each component of the gradient can be very large or very small, thus the diagonal entries of the Hessian matrix, which are per-entry Lipschitz constants of the gradient, can be very large or small. As a result, the Hessian matrix may have a highly dynamic range of diagonal entries, causing a possibly exponentially large condition number. Second, estimating a local Lipschitz constant is too time consuming, thus in practice we often pick a constant step-size or use a fixed step-size schedule. If the Lipschitz constant changes dramatically along the trajectory of the algorithm, then a constant stepsize could be much smaller than the theoretical step-size, thus significantly slowing down the algorithm.

How to resolve the issue of gradient explosion/vanishing? For the 1-dimensional example discussed above, one can choose an initial point inside the basin near the global minimum. Similarly, for a general high-dimensional problem, one solution is to choose an initial point inside a "good basin" that allows the iterates move fast. In the next subsection, we will discuss initialization strategies in detail.

4.2 Careful Initialization.

In the rest of this section, we will discuss three major tricks for training deep neural networks. In this subsection, we discuss the first trick: careful initialization.

As discussed earlier, exploding/vanishing gradient regions indeed exist and occupy a large portion of the whole space, and initializing in these regions will make the algorithm fail. Thus, a natural idea is to pick the initial point in a nice region to start with.

Naive Initialization Since the "nice region" is unknown, the first thought is to try some simple initial points. One choice is the all-zero initial point, and another choice is a sparse initial point that only a small portion of the weights are non-zero. Yet another choice is to draw the weights from certain random distribution. Trying these initial points would be painful as it is not easy to make them always work: even if an initialization strategy works for the current problem, it might fail for other neural network problems. Thus, a principled initialization method is needed.

Random initialization with specific variance. (Bottou initialization or LeCun initialization [4]) Early works in 1980's Bottou [28] and LeCun et al. [110] described an initialization method for neural-nets with sigmoid activation functions as follows:

$$E(W_{ij}^l) = 0, \quad \mathrm{var}(W_{ij}^l) = \frac{1}{d_{l-1}}, \quad l = 1, 2, \ldots, L; i = 1, \ldots, d_{l-1}; j = 1, \ldots, d_l. \tag{15}$$

In other words, the variance of each weight is 1/fan-in, where fan-in is the number of weights fed into the node. Although simple, this is a non-trivial finding. It is not hard to tune the scaling of the random initial point to make it work, but one may find that one scaling factor does not work well for another network. It requires some understanding of neural-nets to realize that adding the dependence on fan-in can lead to a tuning-free initial point.

Pre-training and Xavier initialization. In late 2000's, the revival of neural networks was attributed to pre-training methods that provide good initial point (e.g. [87, 58]). Partially motivated by this trend, Xavier Glorot and Bengio [73] analyzed signal propagation in deep neural networks at initialization, and proposed an initialization method known as Xavier initialization (or Glorot initialization, Glorot normalization):

$$E(W_{ij}^l) = 0, \quad \mathrm{var}(W_{ij}^l) = \frac{2}{d_{l-1} + d_l}, \quad l = 1, 2, \ldots, L; i = 1, \ldots, d_{l-1}; j = 1, \ldots, d_l, \tag{16}$$

or sometimes written as $\mathrm{var}(W_{ij}) = 2/(\text{fan-in} + \text{fan-out})$, where fan-in and fan-out are the input/output dimensions. One example is a Gaussian distribution $W_{ij}^l \sim \mathcal{N}(0, \frac{2}{d_{l-1}+d_l})$, and another example is a uniform distribution $W_{ij}^l \sim \mathrm{Unif}[-\frac{\sqrt{6}}{\sqrt{d_{l-1}+d_l}}, \frac{\sqrt{6}}{\sqrt{d_{l-1}+d_l}}]$.

Xavier initialization can be derived as follows. For feed-forward signal propagation, according to the same argument as Bottou initialization, one could set the variance of the weights to be 1/fan-in. For the backward signal propagation, according to (10), $e^l = (W^{l+1})^T e^{l+1}$ for a linear network. By a similar argument, one could set the variance of the weights to be 1/fan-out. To handle both feedforward and backward signal propagation, a reasonable heuristic is to set $E(w) = 0, \mathrm{var}(w) = 2/(\text{fan-in} + \text{fan-out})$ for each weight, which is exactly (16).

Kaiming initialization. Bottou initialization and Xavier initialization were designed for sigmoid activation functions which have slope 1 in the "'linear regime" of the activation function. ReLU (rectified linear units) activation [74] became popular after 2010, and He et al. [85] noticed that the derivation of Xavier initialization can be modified to better serve ReLU [5]. The intuition is that for a symmetric random variable ξ, $E[\mathrm{ReLU}(\xi)] = E[\max\{\xi, 0\}] = \frac{1}{2}E[\xi]$, i.e., ReLU cuts half of the signal on average. Therefore, they propose a new initialization method

$$E(W_{ij}^l) = 0, \quad \mathrm{var}(W_{ij}^l) = \frac{2}{d_{\mathrm{in}}} \text{ or } \mathrm{var}(W_{ij}^l) = \frac{2}{d_{\mathrm{out}}}. \tag{17}$$

[4]This initialization is sometimes called LeCun initialization, but it appeared first in Page 9 of Bottou [28], as pointed out by Bottou in private communication, so a proper name may be "Bottou-initialization".

[5]Interestingly, ReLU was also popularized by Glorot et al. [74], but they did not apply their own principle to the new neuron ReLU.

LSUV. The previously discussed initialization methods are data-independent, and it is natural to design a data-dependent initialization method. Mishkin and Matas [142] proposed layer-sequential unit-variance (LSUV) initialization that consists of two steps: first, initialize the weights with orthogonal initialization (e.g., see Saxe et al. [175]), then for each mini-batch, normalize the variance of the output of each layer to be 1 by directly scaling the weight matrices. It shows empirical benefits for some problems.

Infinite width networks with general non-linear activations. The derivation of Kaiming initialization cannot be directly extended to general non-linear activations. Even for one dimensional case where $d_i = 1, \forall i$, the output of 2-layer neural network $\hat{y} = \phi(w_2\phi(w_1 x))$ for random weights $w_1, w_2 \in \mathbb{R}$ is a complicated random distribution. To handle this issue, Poole et al. [167] proposed to use mean-field approximation to study infinite-width networks. Roughly speaking, based on the central limit theorem that the sum of a large number of random variables is approximately Gaussian, the pre-activations of each layer are approximately Gaussians, and then they study the evolution of the variance of each layer. Note that this analysis is closely related to neural tangent kernel [91] discussed in Section 6.3.2, which also analyzes infinite-width networks.

Analysis of finite width networks. The analysis of infinite-width networks can explain the experiments on very wide networks, but narrow networks may exhibit different behavior. A rigorous quantitative analysis is given in Hanin and Rolnick [83], which analyzed finite width networks with ReLU activations. Their analysis might be helpful for explaining why training deep networks is difficult (note that there are other conjectures on the training difficulty of deep networks; e.g. [157]).

Dynamical isometry. Another line of research that aims to understand signal propagation is based on the notion of dynamical isometry [175]. It means that the input-output Jacobian (defined below) has *all* singular values close to 1. Consider a neural-net $f(x) = \phi(W^L\phi(W^{L-1}\dots\phi(W^1 x)))$, which is slightly different from (1) (with an extra ϕ at the last layer). Its "input-output Jacobian" is

$$\frac{\partial z^L}{\partial z^0} = \Pi_{l=1}^{L}(D^l W^l),$$

where D^l is a diagonal matrix with entries being the elements of $\phi'(h_1^l, \dots, h_{d_l}^l)$.

Saxe et al. [175] studied orthogonal initialization for deep linear networks. A formal analysis for deep non-linear networks with infinite width was provided in Pennington et al. [164, 165]. They used tools from free probability theory to compute the distribution of all singular values of the input-output Jacobian (more precisely, the limiting distribution as the width goes to infinity). An interesting discovery is that dynamical isometry can be achieved when using sigmoid activation and orthogonal initialization, but cannot be achieved for Gaussian initialization. Note that one needs to carefully pick σ_w^2, σ_b^2 and $\|x\|^2$, and simply using orthogonal initialization is not enough, which partially explains why Saxe et al. [175] did not observe the benefit of orthogonal initialization.

Dynamical isometry for CNN. One obstacle of applying orthogonal initialization to practical networks is convolution operators: it is not clear at all how to compute an "orthogonal" convolution operator. Xiao et al. [215] proposed two orthogonal initialization methods for CNN, and the simpler and better version DeltaOrthogonal initialization is available in standard deep learning libraries. With DeltaOrthogonal initialization, they can train a 10000-layer CNN without other tricks like batch-normalization or skip connections (these tricks are discussed later).

Dynamical isometry for other networks. The analysis of dynamical isometry has been applied to other neural networks as well. Li and Nguyen [117] analyzed dynamical isometry for deep autoencoders, and showed that it is possible to train a 200-layer autoencoder without tricks like layer-wise pre-training and batch normalization. Gilboa et al. [72] analyzed dynamical isometry for LSTM and RNNs, and proposed a new initialization scheme that performs much better than traditional initialization schemes in terms of reducing training instabilities.

Meta-initialization. Dauphin and Schoenholz [42] proposed another data-dependent initialization method. Their intuition is that a good initialization makes gradient descent easier by starting in regions that "look locally linear with minimal second order effects". They proposed a quantitative measure called "gradient quotient" that formalizes this intuition, and used an additional optimization algorithm that finds an initial point with small gradient quotient. [42] used DeltaOrthogonal initialization as s a starting point and used its meta-initialization method to find a better initial point. The found initial point can achieve the state-of-the-art result, without using normalization methods.

4.3 Normalization Methods

The second approach is normalization during the algorithm. This can be viewed as an extension of the first approach: instead of merely modifying the initial point, this approach modifies the network for all the following iterates. One representative method is batch normalization (BatchNorm) [90], which is a standard technique nowadays.

Essence of BatchNorm. The goal of BatchNorm is to normalize the output at each layer across samples. The essence of BatchNorm method in [90] is to view the normalization step as a nonlinear transformation "BN" and add BN layers to the original neural network. BN layers play the same role as the activation function ϕ and other layers (such as max pooling layers). This modification can be consistent with BP as long as the chain rule of the gradient can be applied, or equivalently, the gradient of this operation BN can be computed. Note that a typical optimization-style solution would be to add constraints that encode the requirements; in contrast, the solution of BN is to add a non-linear transformation to encode the requirements. This is a typical neural-net style solution.

Understanding BatchNorm. The original BatchNorm paper claims that BatchNorm reduces the "internal covariate shift". Santurkar et al. [174] argues that internal covariate shift has little do with the success of BatchNorm, and the major benefit of BatchNorm is to reduce the Lipschitz constants (of the objective and the gradients). Bjorck et al. [25] shows that the benefit of BatchNorm is to allow larger learning rate, and discusses the relation with initialization schemes. Arora et al. [12], Cai et al. [34], Kohler et al. [105] analyzed the theoretical benefits of BatchNorm (mainly larger or auto-tuning learning rate) under various settings. Ghorbani et al. [71] numerically found that for networks without BatchNorm, there are large isolated eigenvalues, while for networks with BatchNorm this phenomenon does not occur.

Other normalization methods. One issue of BatchNorm is that the mean and the variance for each mini-batch is computed as an approximation of the mean/variance for all samples, thus if different mini-batches do not have similar statistics then BN does not work very well. Researchers have proposed other normalization methods such as weight normalization [173], layer normalization [13], instance normalization [200], group normalization [214] and spectral normalization [143] and switchable normalization [132].

4.4 Changing Neural Architecture

The third approach is to change the neural architecture. Around 2014, people noticed that from AlexNet [106] to Inception [193], the neural networks get deeper and the performance gets better, thus it is natural to further increase the depth of the network. However, even with smart initialization and BatchNorm, people found training more than 20-30 layers is very difficult. As shown in [86], for a given network architecture VGG, a 56-layer network achieves worse training and test accuracy than a 20-layer network [6]. Thus, a major challenge at that time was to make training an "ultra-deep" neural network possible.

ResNet. The key trick of ResNet [86] is simple: adding an identity skip-connection for every few layers. More specifically, ResNet changes the network from (2) to

$$z^0 = x; z^l = \phi(\mathcal{F}(W^l, z^{l-1}) + z^{l-1}), \quad l = 1, \dots, L, \tag{18}$$

where $\mathcal{F}$ represents a few layers of the original networks, such as $\mathcal{F}(W_1, W_2, z) = W_1\phi(W_2 z)$. Note that a commonly seen expression of ResNet (especially in theoretical papers) is $z^l = \mathcal{F}(W^l, z^{l-1}) + z^{l-1}$, which does not have the extra $\phi(\cdot)$, but (18) is the form used in practical networks. Note that the expression (18) only holds when the input and output have the same dimension; to change the dimension across layers, one could use extra projection matrices (i.e. change the second term z^{l-1} to $U^l z^{l-1}$) or use other operations (e.g. pooling). In theoretical analysis, the form of (18) is often used.

ResNet has achieved remarkable success: with the simple trick of adding identity skip connection (and also BatchNorm), ResNet with 152 layers greatly improved the best test accuracy at that time for a few computer vision tasks including ImageNet classification (improving top-5 error to a remarkable result 3.57%).

Other architectures. Neural architecture design is one of the major threads of current deep learning research. Other popular architecture related to ResNet include high-way networks [190], DenseNet [89] and ResNext [216]. While these architectures are designed by humans, another recent trend is the automatic search of neural architectures (neural architecture search) [240]. There are also intermediate approaches: search one or few hyper-parameters of the neural-architecture such

[6] Note that this difficulty is probably not due to gradient explosion/vanishing, and perhaps related to singularities [157].

as the width of each layer [224, 195]. Currently, the state-of-the-art architectures (e.g. EfficientNet [195]) for ImageNet classification can achieve much higher top-1 accuracy than ResNet (around 85% v.s. 78 %) with the aid of a few extra tricks.

Analysis of ResNet and initialization. Understanding the theoretical advantage of ResNet or skip connections has attracted much attention. The benefits of skip connections are likely due to multiple factors, including better generalization ability (or feature learning ability), better signal propagation and better optimization landscape. For instance, Orhan and Pitkow [157] suggests that skip connections improve the landscape by breaking symmetry.

Following the theme of this section on signal propagation, we discuss some results on the signal propagation aspects of ResNet. As mentioned earlier, Hanin [82] discussed two failure modes for training; in addition, it proved that for ResNet if failure mode 1 does not happen then failure mode 2 does not happen either. Tarnowski et al. [196] proved that for ResNet, dynamic isometry can be achieved for any activation (including ReLU) and any bi-unitary random initialization (including Gaussian and Orthogonal initialization). In contrast, for the original (non-residual) network, dynamic isometry is achieved only for orthogonal initialization and certain activations (excluding ReLU).

Besides theoretical analysis, some works further explored the design of new initialization schemes such as [219, 15, 231]. Yang and Schoenholz [219] analyzed randomly initialized ResNet and showed that the optimal initial variance is different from Xavier or He initialization and should depend on the depth. Balduzzi et al. [15] analyzed ResNet with recursion $z^{l+1} = z^l + \beta W^l \cdot \mathrm{ReLU}(z^l)$, where β is a scaling factor. It showed that for β-scaled ResNet with BatchNorm and Kaiming intialization, the correlation of two input vectors scales as $\frac{1}{\beta\sqrt{L}}$, thus it suggests a scaling factor $\beta = 1/\sqrt{L}$. Zhang et al. [231] analyzed the signal propagation of ResNet carefully, and proposed Fixup initialization which leads to good performance on ImageNet, without using BatchNorm.

4.5 Training Ultra-Deep Neural-nets

There are a few approaches that can currently train very deep networks (say, more than 1000 layers) nowadays to reasonable test accuracy for image classification tasks.

- The most well-known approach uses all three tricks discussed above (or variants): proper initialization, proper architecture (e.g. ResNet) and BatchNorm.
- Using FixUp initialization or meta-initialization [42]) in ResNet [7] [231].
- Only using a carefully chosen initial point such as orthogonal initialization [215], without the help of normalization methods or ResNet.

Besides the three tricks discussed in this section, there are quite a few design choices that are probably important for achieving good performance of neural networks. These include but not

[7] Note that these two papers also uses a certain scalar normalization trick that is much simpler than BatchNorm.

limited to data processing (data augmentation, adversarial training, etc.), optimization methods (optimization algorithms, learning rate schedule, learning rate decay, etc.), regularization (ℓ_2-norm regularization, dropout, etc.), neural architecture (depth, width, connection patterns, filter numbers, etc.) and activation functions (ReLU, leaky ReLU, ELU, tanh, swish, etc.). We have only discussed three major design choices which are relatively well understood in this section. We will discuss a few other choices in the following sections, mainly the optimization methods and the width.

5 General Algorithms for Training Neural Networks

In the previous section, we discussed neural-net specific tricks. These tricks need to be combined with an optimization algorithm such as SGD, and are largely orthogonal to optimization algorithms. In this section, we discuss optimization algorithms used to solve neural network problems, which are often generic and can be applied to other optimization problems as well.

For a more detailed tutorial of standard methods for machine learning (not just deep learning), see Bottou, Curtis and Nocedal [30] and Curtis and Scheinberg [41]

5.1 SGD and learning-rate schedules

We can write (3) as a finite-sum optimization problem:

$$\min_{\theta} F(\theta) \triangleq \frac{1}{B} \sum_{i=1}^{B} F_i(\theta). \tag{19}$$

Each $F_i(\theta)$ represents the sum of training loss for a mini-batch of training samples (e.g. 32, 64 or 512 samples), and B is the total number of mini-batches (smaller than the total number of training samples n). The exact expression of F_i does not matter in this section, as we only need to know how to compute the gradient $\nabla F_i(\theta)$.

Currently, the most popular class of methods are SGD and its variants. Theoretically, SGD works as follows: at the t-th iteration, randomly pick i and update the parameter by

$$\theta_{t+1} = \theta_t - \alpha_t \nabla F_i(\theta_t).$$

In practice, the set of all samples are randomly shuffled at the beginning of each epoch, then split into multiple mini-batches. At each iteration, one mini-batch is loaded into the memory for computation (computing mini-batch gradient and performing weight update).

Vanilla learning rate schedules. Similar to the case in general nonlinear programming, the choice of step-size (learning rate) is also important in deep learning. In the simplest version of SGD, constant step-size $\alpha_t = \alpha$ works reasonably well: it can achieve a very small training error and relatively small test error for many common datasets. Another popular version of SGD is to divide the step-size by a fixed constant once every few epochs (e.g. divide by 10 every 5-10 epochs) or divide by a constant when stuck. Some researchers refer to SGD with such simple steps-size update rule as ”vanilla SGD”.

Learning rate warmup. “Warmup” is a commonly used heuristic in deep learning. It means to use a very small learning rate for a number of iterations, and then increases to the “regular” learning rate. It has been used in a few major problems, including ResNet [86], large-batch training for image classification [78], and many popular natural language architectures such as Transformer networks [201] BERT [47]. See Gotmare et al. [77] for an empirical study of warmup.

Cyclical learning rate. An interesting variant is SGD with cyclical learning rate ([184, 129]). The basic idea is to let the step-size bounce between a lower threshold and an upper threshold. In one variant called SGDR (Smith [184]), the general principle is to gradually decrease and then gradually increase step-size within one epoch, and one special rule is to use piecewise linear step-size. A later work [185] reported “super convergence behavior” that SGDR converges several times faster than SGD in image classification. In another variant of Ioshchilov et al. [129], within one epoch the step-size gradually decreases to the lower threshold and *suddenly* increases to the upper threshold (”restart”). This “restart” strategy resembles classical optimization tricks in, e.g., Powell [168] and O’Donoghue and Candes [155]. Gotmare et al. [77] studied the reasons of the success of cyclical learning rates, but a thorough understanding remains elusive.

5.2 Theoretical analysis of SGD

In the previous subsection, we discussed the learning rate schedules used in practice; next, we discuss the theoretical analysis of SGD. The theoretical convergence of SGD has been studied for decades (e.g., [133]). For a detailed description of the convergence analysis of SGD, we refer the readers to Bottou et al. [30]. However, there are at least two issues of the classical analysis. First, the existing analysis assumes Lipschitz continuous gradients similar to the analysis of GD, which cannot be easily justified as discussed in Section 3.2. We put this issue aside, and focus on the second issue that is specific to SGD.

Constant v.s. diminishing learning rate. The existing convergence analysis of SGD often requires diminishing step-size , such as $\eta_t = 1/t^{\alpha}$ for $\alpha \in (1/2, 1]$ [133, 30]. Results for SGD with constant step-size also exist (e.g., [30, Theorem 4.8]), but the gradient does not converge to zero since there is an extra error term dependent on the step-size. This is because SGD with constant stepsize may finally enter a “confusion zone” in which iterates jump around [133]. Early works in deep learning (e.g. LeCun et al. [110]) suggested using diminishing learning rate such as $O(1/t^{0.7})$, but nowadays constant learning rate works quite well in many cases. For practitioners, this unrealistic assumption on the learning rate makes it harder to use the theory to guide the design of the optimization algorithms. For theoreticians, using diminishing step-size may lead to a convergence rate far from practical performance.

New analysis for constant learning rate: realizable case. Recently, an explanation of the constant learning rate has become increasingly popular: if the problem is realizable (the global optimal value is zero), then SGD with constant step-size does converge [177, 202] [8]. In other words, if the network is powerful enough to represent the underlying function, then the stochastic noise causes little harm in the final stages of training, i.e., realizability has an "automatic variance reduction" effect [126]. Note that "zero global minimal value" is a strong assumptions for a general unconstrained optimization problem, but the purpose of using neural networks is exactly to have strong representation power, thus "zero global minimal value" is a reasonable assumption in deep learning. This line of research indicates that neural network optimization has special structure, thus classical optimization theory may not provide the best explanations for neural-nets.

Acceleration over GD. We illustrate why SGD is faster than GD by a simple realizable problem. Consider a least squares problem $\min_{w \in \mathbb{R}^d} \frac{1}{2n} \sum_{i=1}^{n} (y_i - w^T x_i)^2$, and assume the problem is realizable, i.e., the global minimal value is zero. For simplicity, we assume $n \geq d$, and the data are normalized such that $\|x_i\| = 1, \forall i$. It can be shown (e.g. [202, Theorem 4]) that the convergence rate of SGD with learning rate $\eta = 1$ is $\frac{n}{d} \frac{\lambda_{\max}}{\lambda_{\text{avg}}}$ times better than GD, where $\lambda_{\max}$ is the maximum eigenvalue of the Hessian matrix $\frac{1}{n} X X^T$ and λ_{avg} is the average eigenvalue of the same matrix. Since $1 \leq \frac{\lambda_{\max}}{\lambda_{\text{avg}}} \leq d$, the result implies that SGD is n/d to n times faster than GD. In the extreme case that all samples are almost the same, i.e., $x_i \approx x_1, \forall\, i$, SGD is about n times faster than GD (this simple example was pointed out by, e.g., Bottou [29]). In the above analysis, we assume each mini-batch consists of a single sample. When there are N mini-batches, SGD is roughly 1 to N times faster than GD. In practice, the acceleration ratio of SGD over GD depends on many factors, and the above analysis can only provide some preliminary insight for understanding the advantage of SGD.

5.3 Momentum and accelerated SGD

Another popular class of methods are SGD with momentum and SGD with Nesterov momentum. SGD with momentum works as follows: at the t-th iteration, randomly pick i and update the momentum term and the parameter by

$$m_t = \beta m_{t-1} + (1 - \beta) \nabla F_i(\theta_t); \quad \theta_{t+1} = \theta_t - \alpha_t m_t.$$

We skip the expression of SGD with Nesterov momentum here (see, e.g., [171]).

They are the stochastic versions of the heavy-ball method and accelerated gradient method, but are commonly rebranded as "momentum methods" in deep learning. They are widely used in machine learning area not only because of faster speed than vanilla SGD in practice, but also because of the theoretical advantage for convex or quadratic problems. In particular, heavy-ball method achieves a better convergence rate than vanilla GD for convex quadratic functions, and Nesterov's accelerated gradient method achieves a better convergence rate for convex functions; see Appendix A for more detailed discussions.

[8] Rigorously speaking, the conditions are stronger than realizability (e.g. weak growth condition in [202]). For certain problems such as least squares, realizablity is enough since it implies the weak growth condition in [202].

Theoretical advantage of SGD with momentum. The classical results on the benefit of momentum only apply to the batch methods (i.e. all samples are used at each iteration). It is interesting to understand whether momentum can improve the speed of the stochastic version of GD in theory. Unfortunately, even for convex problems, achieving such a desired acceleration is not easy according to various negative results (e.g. [49, 48, 103]). For instance, Kidambi et al. [103] showed that there are simple quadratic problem instances that momentum does not improve the convergence speed of SGD. Note that this negative result of [103] only applies to the naive combination of SGD and momentum terms for a general convex problem.

There are two ways to obtain better convergence rate than SGD. First, by exploiting tricks such as variance reduction, more advanced optimization methods (e.g. [124, 2]) can achieve an improved convergence rate that combines the theoretical improvement of both momentum and SGD. However, these methods are somewhat complicated, and are not that popular in practice. Defazio and Bottou [45] analyzed the reasons why variance reduction is not very successful in deep learning. Second, by considering more structure of the problem, simpler variants of SGD can achieve acceleration. Jain et al. [92] incorporated statistical assumption of the data to show that a certain variant is faster than SGD. Liu and Belkin [125] considered realizable quadratic problems, and proposed a modified version of SGD with Nesterov's momentum which is faster than SGD.

Accelerated SGD for non-convex problems. The above works only apply to convex problems and are thus not directly applicable to neural network problems which are *non-convex*. Designing accelerated algorithms for general non-convex problems is quite hard: even for the batch version, accelerated gradient methods cannot achieve better convergence rate than GD when solving non-convex problems. There have been many recent works that design new methods with faster convergence rate than SGD on general non-convex problems (e.g. [36, 35, 217, 59, 3] and references therein). These methods are mainly theoretical and not yet used by practitioners in deep learning area. One possible reason is that they are designed for worst-case non-convex problems, and do not capture the structure of neural network optimization.

5.4 Adaptive gradient methods: AdaGrad, RMSProp, Adam and more

The third class of popular methods are adaptive gradient methods, such as AdaGrad [57], RMSProp [199] and Adam [104]. We will present these methods and discuss their empirical performance and the theoretical results.

Descriptions of adaptive gradient methods. AdaGrad works as follows: at the t-th iteration, randomly pick i, and update the parameter as (let $\circ$ denote entry-wise product)

$$\theta_{t+1} = \theta_t - \alpha_t v_t^{-1/2} \circ g_t, \quad t = 0, 1, 2, \ldots, \tag{20}$$

where $g_t = \nabla F_i(\theta_t)$ and $v_t = \sum_{j=1}^{t} g_j \circ g_j$. In other words, the step-size for the k-th coordinate is adjusted from α_t in standard SGD to $\alpha_t / \sqrt{\sum_{j=0}^{t} g_{j,k}^2}$ where $g_{j,k}$ denotes the k-th entry of g_j.

One drawback of AdaGrad is that it treats all past gradients equally, and it is thus natural to use exponentially decaying weights for the past gradients. This new definition of v_t leads to another algorithm RMSProp [199] (and a more complicated algorithm AdaDelta [229]; for simplicity, we only discuss RMSProp). More specifically, at the t-th iteration of RMSProp, we randomly pick i and compute $g_t = \nabla F_i(\theta_t)$, and then update the second order momentum v_t and parameter θ_t as

$$\begin{aligned} v_t &= \beta v_{t-1} + (1-\beta) g_t \circ g_t, \\ \theta_{t+1} &= \theta_t - \alpha_t v_t^{-1/2} \circ g_t. \end{aligned} \tag{21}$$

Adam [104] is the combination of RMSProp and the momentum method (i.e. heavy ball method). At the t-th iteration of RMSProp, we randomly pick i and compute $g_t = \nabla F_i(\theta_t)$, and then update the first order momentum m_t, the second order momentum v_t and parameter θ_t as

$$\begin{aligned} m_t &= \beta_1 m_{t-1} + (1-\beta_1) g_t, \\ v_t &= \beta_2 v_{t-1} + (1-\beta_2) g_t \circ g_t, \\ \theta_{t+1} &= \theta_t - \alpha_t v_t^{-1/2} \circ m_t. \end{aligned} \tag{22}$$

There are a few other related methods in the area, e.g. AdaDelta [229], Nadam [52], and interested readers can refer to [171] for more details.

Empirical use of adaptive gradient methods. AdaGrad was designed to deal with sparse and highly unbalanced data. Imagine we form a data matrix with the data samples being the columns, then in many machine learning applications, most rows are sparse (infrequent features) and some rows are dense (frequent features). If we use the same learning rate for all coordinates, then the infrequent coordinates will be updated too slowly compared to frequent coordinates. This is the motivation to use different learning rates for different coordinates. AdaGrad was later used in many machine learning tasks with sparse data such as language models where the words have a wide range of frequencies [141, 163].

Adam is one of the most popular methods for neural network training nowadays [9]. After Adam was proposed, the common conception was that Adam converges faster than vanilla SGD and SGD with momentum, but generalizes worse. Later, researchers found that (e.g., [211]) well-tuned SGD and SGD with momentum outperform Adam in both training error and test error. Thus the advantages of Adam, compared to SGD, are considered to be the relative insensitivity to hyperparameters and rapid initial progress in training (see, e.g. [101]). Sivaprasad et al. [183] proposed a metric of "tunability" and verified that Adam is the most tunable for most problems they tested.

The claim of the "marginal value" of adaptive gradient methods [211] in year 2017 did not stop the booming of Adam in the coming years. Less tuning is one reason, but we suspect that another reason is that the simulations done in [211] are limited to image classification, and do not reflect

[9] The paper that proposed Adam [104] achieved phenomenal success at least in terms of popularity. It was posted in arxiv on December 2014; by Aug 2019, the number of citations in Google scholar is 26000; by Dec 2019, the number is 33000. Of course the contribution to optimization area cannot just be judged by the number of citations, but the attention Adam received is still quite remarkable.

the real application domains of Adam such as GANs and reinforcement learning. For these tasks, the generalization ability of Adam might be a less critical issue.

Theoretical results on adaptive gradient methods. Do these adaptive gradient methods converge? Although Adam is known to be convergent in practice and the original Adam paper [104] claimed a convergence proof, it was recently found in Reddi et al. [169] that RMSProp and Adam can be divergent even for solving convex problems (thus there is some error in the proof of [104]). To fix the divergence issue, [169] proposed AMSGrad, which changes the update of v_t in Adam to the following:

$$\bar{v}_t = \beta_2 \bar{v}_{t-1} + (1 - \beta_2) g_t^2, \quad v_t = \max\{v_{t-1}, \bar{v}_t\}.$$

They also prove the convergence of AMSGrad for convex problems (for diminishing β_1). Empirically, AMSGrad is reported to have somewhat similar (or slightly worse) performance to Adam.

The convergence analysis and iteration complexity analysis of adaptive gradient methods are established for non-convex optimization problems in a few subsequent works [38, 236, 242, 44, 243, 208]. For example, [38] considers a general Adam-type methods where v_t can be any function of past gradients $g_1, \ldots, g_t$ and establishes a few verifiable conditions that guarantee the convergence for non-convex problems (with Lipschitz gradient). We refer interested readers to Barakat and Bianchi [16] which provided a table summarizing the assumptions and conclusions for adaptive gradient methods. Despite the extensive research, there are still many mysteries about adaptive gradient methods. For instance, why it works so well in practice is still largely unknown.

5.5 Large-scale distributed computation

An important topic in neural network optimization is how to accelerate training by using multiple machines. This topic is closely related to distributed and parallel computation (for readers interested in this topic, we recommend the book Bertsekas and Tsitsiklis [24]).

Training ImageNet in 1 hour. Goyal et al. [78] successfully trained ResNet50 (50-layer ResNet) for the ImageNet dataset in 1 hour using 256 GPUs; in contrast, the original implementation in He et al. [86] takes 29 hours using 8 GPUs. The scaling efficiency is $29/32 \approx 0.906$, which is remarkable. Goyal et al. [78] used 8192 samples in one mini-batch, while He et al. [86] only used 256 samples in one mini-batch. Bad generalization was considered to be a major issue for large mini-batches, but [78] argued that optimization difficulty is the major issue. They used two major optimization tricks: first, they scale the learning rate with the size of the mini-batches; second, they use "gradual warmup" strategy that increases the learning rate from η/K gradually to η in the first 5 epochs, where K is the number of machines.

Training ImageNet in minutes. Following Goyal et al. [78], a number of works [186, 1, 96, 140, 222, 218] have further reduced the total training time by using more machines. For example, You et al. [223] applied layer-wise adaptive rate scheduling (LARS) to train ImageNet with mini-batch size 32,000 in 14 minutes. Yamazaki et al. [218] used warmup and LARS, tried many learning rate decay rules and used label smoothing to train ImageNet in 1.2 minutes by 2048 V100 GPUs, with mini-batch size 81920. When training ResNet50 on ImageNet, these works can obtain top-1 test accuracy between 75% to 77%, which is quite close to the single-machine training.

5.6 Other Algorithms

Other learning rate schedules. We have discussed cyclical learning rate and adaptive learning rate. Adaptive stepsize or tuning-free step-size has been extensively studied in non-linear optimization area (see, e.g. Yuan [226] for an overview). One of the representative methods is Barzilai-Borwein (BB) method proposed in year 1988 [19]. Interestingly, in machine learning area, an algorithm with similar idea to BB method (diagonal approximation of Hessian) was proposed in the same year 1988 in Becker et al. [20] (and further developed in Bordes et al. [27]). This is not just a coincidence: it reflects the fact that the problems neural-net researchers have been trying to solve are very similar to those of non-linear optimizers. LeCun et al. [111] provided a good overview of the tricks for training SGD, especially step-size tuning based on the Hessian information. Other recent works on tuning-free SGD include Schaul [176], Tan et al. [194] and Orabona [156].

Second order methods. Second-order methods have also been extensively studied in the neural network area. Along the line of classical second-order methods, Martens [135] presented Hessian-free optimization algorithms, which are a class of quasi-Newton methods without explicit computation of an approximation of the Hessian matrix (thus called "Hessian free"). One of the key tricks, based on [162, 178], is how to compute Hessian-vector products efficiently by backpropagation, without computing the full Hessian. Berahas [22] proposed a stochastic quasi-Newton method for solving neural network problems. Another tye of second order method is the natural gradient method [6, 136], which scales the gradient by the empirical Fisher information matrix (based on theory of information geometry [5]). We refer the readers to [136] for a nice interpretation of natural gradient method and the survey [30] for a detailed introduction. A more efficient version K-FAC, based on block-diagonal approximation and Kronecker factorization, is proposed in Martens and Grosse [137].

Very recently, second order methods showed some promise. Osawa et al. [158] has achieved good test performance on ImageNet using K-FAC (only takes 35 epochs to achieve 75% top-1 accuracy on ImageNet). Anil et al. [7] proposed an efficient implementation of a second-order method Shampoo (Shampoo was proposed in Gupta et al. [79]). It showed that when using Transformer network to solve natural language processing tasks, their method used 40% less wall-clock time compared to first-order methods.

6 Global Optimization of Neural Networks (GON)

The previous two sections mainly focus on resolving "local issues" of training, and the theoretical results can at most ensure convergence to local minima. Due to non-convexity of the problem (3), failure of convergence to global-min has been considered as a major challenge of neural-net training.

Nevertheless, the recent success of neural networks suggest that neural-net optimization is far from a worst-case non-convex problem, and finding a global minimum is not a surprise in deep learning noways. There is a growing list of literature devoted to understanding the global issues of training. Typical questions include but are not limited to: When can an algorithm converge to global minima? Are there sub-optimal local minima? What properties do the optimization landscape have? How to pick an initial point that ensures convergence to global minima?

For simplicity of presentation, we call this subarea "global optimization of neural networks" (GON) [10]. We remark that research in GON was partially reviewed in Vidal et al. [206], but most of the works we reviewed appear after [206].

6.1 Related areas

Before discussing neural networks, we discuss a few related subareas.

Tractable problems. Understanding the boundary between "tractable" and "intractable" problems has been one of the major themes of optimization area. The most well-known boundary is probably between convex and non-convex problems. However, this boundary is vague since it is also known that many non-convex optimization problems can be reformulated as a convex problem (e.g. semi-definite programming and geometric programming). We guess that some neural-net problems are in the class of "tractable" problems, though the meaning of tractability is not clear. Studying neural networks, in this sense, is not much different in essence from the previous studies of semi-definite programming (SDP), except that a theoretical framework as complete as SDP has not been developed yet.

Global optimization. Another related area is "global optimization", a subarea of optimization which aims to design and analyze algorithms that find globally optimal solutions. The topics include global search algorithms for general non-convex problems (e.g. simulated annealing and evolutionary methods), algorithms designed for specific non-convex problems (possibly discrete; e.g. [130]), as well as analysis of the structure of specific non-convex problems (e.g. [61]).

Non-convex matrix/tensor factorization. The most related subarea to GON is "non-convex optimization for matrix/tensor factorization" (see, e.g., Chi et al. [39] for a survey), which emerged after around year 2009 in machine learning and signal processing areas [11]. This subarea tries to understand why many non-convex matrix/tensor problems can be solved to global minima easily. Most of these problems can be viewed as the extensions of matrix factorization problem

$$\min_{X,Y \in \mathbb{R}^{n\times r}} \|M - XY^T\|_F^2, \tag{23}$$

including low-rank matrix completion, phase retrieval, matrix sensing, dictionary learning and tensor decomposition. The matrix factorization problem (23) is closely related to the eigenvalue

[10]It is not clear how we should call this subarea. Many researchers use "(provable) non-convex optimization" to distinguish these research from convex optimization. However, this name may be confused with the studies of non-convex optimization that focus on the convergence to stationary points. The name "global optimization" might be confused with research on heuristic methods, while GON is mainly theoretical. Anyhow, let's call it global optimization of neural-nets in this article.

[11]Again, it is not clear how to call this subarea. "Non-convex optimization" might be a bit confusing to optimizers.

problem. Classical linear algebra textbooks explain the tractability of the (original) eigenvalue problem by proving directly the convergence of power method, but it cannot easily explain what happens if a different algorithm is used. In contrast, an optimization explanation is that the eigenvalue problem can be solved to global optima because every local-min is a global-min. One central theme of this subarea is to study whether a nice geometrical property still holds for a variant of (23). This is similar to GON area, which essentially tries to understand the structure of deep non-linear neural-nets that also can be viewed as a generalized formulation of (23).

6.2 Empirical exploration of landscape

We first discuss some interesting empirical studies on the loss surface of neural networks. The loss surface is a high-dimensional surface $(\theta, F(\theta))$ in $\mathbb{R}^{D+1}$, where D is the total number of parameters, and is also called "optimization landscape" or "landscape". Theoretical results will be reviewed in later subsections.

One of the early papers that caught much attention is Dauphin et al. [43], which showed that empirically bad local minima are not found and a bigger challenge is plateaus. Goodfellow et al. [76] plotted the function values along the line segment between the initial point and the converged point, and found that this 1-dimensional plot is similar to a 1-dimensional convex plot which has no bumps. These early experiments indicated that the landscape of a neural-net problem is much nicer than one thought.

A few later works provided various ways to explore the landscape. Poggio and Liao [166] gave experiments on the visualization of the evolution of SGD. Li et al. [116] provided visualization of the landscape under different network architecture. In particular, it showed by two-dimensional visualization that as the width increases, then landscape becomes "smoother", and adding skip connection will also smooth the landscape. Baity-Jesi et al. [14] compared the learning dynamics of neural-nets with glassy systems in statistical physics. Franz et al. [64] and Geiger et al. [70] studied the analogy between the landscape of neural networks and the jamming transition in physics.

6.2.1 Mode connectivity

An exact characterization of a high-dimensional surface is almost impossible, thus in mathematics, geometers strive to identify simple yet non-trivial properties (e.g. Gauss's curvature). In neural-net area, one geometrical property called "mode connectivity" has been found for deep neural networks. In particular, Draxler et al. [53] and Garipov et al. [67] independently found that two global minima can be connected by an (almost) equal-value path. This is an empirical claim, and in practice the two "global minima" refer to two low-error solutions found by training from two random initial points. A more general optimization property is "connectivity of sub-level sets", which was first proved by [65] for 1-hidden layer linear networks, and further justified in Nguyen [150], Kuditipudi et al. [107] for multi-layer neural nets.

6.2.2 Model compression and lottery ticket hypothesis

Another line of research closely related to the landscape is training smaller neural networks (or called "efficient deep learning"). This line of research has a close relation with GON, and this relation has been largely ignored by both theoreticians and practitioners.

Network pruning [81] showed that many large networks can be pruned to obtain a much smaller network while the test accuracy is only dropped little. Nevertheless, in network pruning, the small network often has to inherit the weights from the solution found by training the large network to achieve good performance, and training a small network from the scratch often leads to significantly worse performance [12].

Frankle and Carbin [62] made an interesting finding that in some cases a good initial point is relatively easy to find. More specifically, for some datasets (e.g. CIFAR10), [62] empirically shows that a large network contains a small subnetwork and a certain "half-random" initial point such that the following holds: training the small network from this initial point can achieve performance similar to the large network. The trainable subnetwork (the architecture and the associated initial point together) is called a "winning ticket", since it has won an "initialization lottery". Lottery ticket hypothesis (LTH) states that such a winning ticket always exists. Later work [63] shows that for larger datasets such as ImageNet, the procedure in [62] needs to be modified to find a good initial point. Zhou et al. [237] further studies the factors that lead to the success of the lottery tickets (e.g. the signs of the weights are very important). For more discussions on LTH, see Section 3.1 of [145].

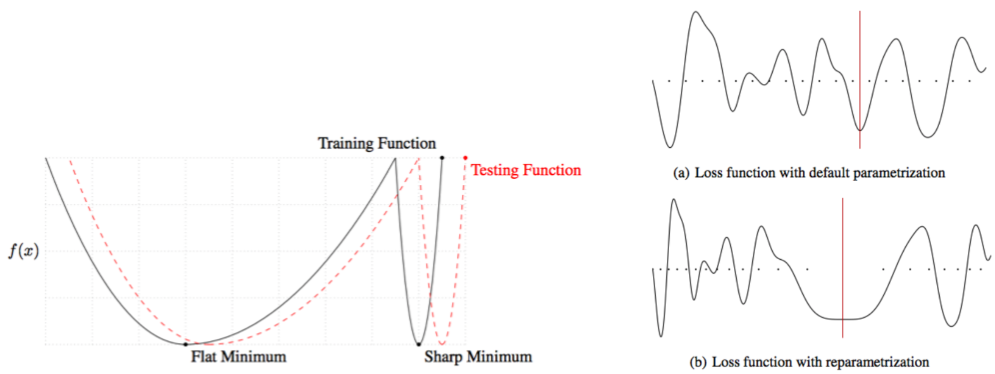
The works on network pruning and LTH are mostly empirical, and a clean message is yet to be stated due to the complication of experiments. It is an interesting challenge to formally state and theoretically analyze the properties related to model compression and LTH. Tian et al. [198] made an attempt on a more formal analysis of LTH in one-hidden-layer networks. More theoretical works along this line are needed.

6.2.3 Generalization and landscape

Landscape has long been considered to be related to the generalization error. A common conjecture is that flat and wide minima generalize better than sharp minima, with numerical evidence in, e.g., Hochreiter and Schmidhuber [88] and Keskar et al. [102]. The intuition is illustrated in Figure 2(a): the test loss function and the training loss function have a small difference, and that difference has a small effect on wide minima and thus they generalize well; in constrast, this small difference has a large effect on sharp minima and thus they do not generalize well. Dinh et al. [51] argues that sharp minima can also generalize since they can become wide minima after re-parameterization; see Figure 2(b). How to define "wide" and "sharp" in a rigorous way is still challenging. Neyshabur et al. [147], Yi et al. [221] defined new metrics for the "flatness" and showed the connection between

[12] There are some recent pruned networks that can be trained from random initial point [127, 113], but the sparsity level is not very high; see [63, Appendix A] for discussions.

generalization error and the new notions of "flatness". He et al. [84] found that besides wide and shallow local minima, there are asymmetric minima that the function value changes rapidly along some direction and slowly along some other directions, and algorithms biased towards the wide side generalize better.



(a) Wide minima generalize better [102]

(b) Sharp minima may become wide after re-parameterization [51]

Figure 2: Illustration on wide minima and sharp minima.

Although the intuition "wide minima generalize better" is debatable, researchers still borrow this intuition to design or discuss optimization algorithms. Chaudhari et al. [37] designed entropy-SGD that explicitly search for wider minima. Smith and Topin [185] also argued that the benefit of cyclical learning rate is that it can escape shallow local minima

6.3 Optimization Theory for Deep Neural Networks

We discuss two recent threads in optimization theory for *deep* neural networks: landscape analysis and algorithmic analysis. The first thread discusses the global landscape properties of the loss surface, and the second thread mainly analyzes gradient descent for ultra-wide networks.

6.3.1 Global landscape analysis of deep networks

Global landscape analysis is the closest in spirit to the empirical explorations in Section 6.3: understanding some geometrical properties of the landscape. There are three types of deep neural networks with positive results so far: linear networks, over-parameterized networks and modified networks. We will also discuss some negative results.

Deep linear networks. Linear networks have little representation power and are not very interesting from a learning perspective, but it is a valid problem from optimization perspective. The landscape of deep linear networks are relatively well understood. Kawaguchi [99] proved that every local-min is a global-min for a deep linear networks, under very mild conditions. Lu and

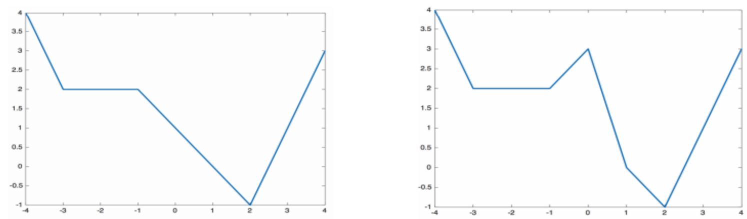


Figure 3: Left figure: the flat region is not a set-wise strict local-min, and this region can be escaped by a (non-strictly) decreasing algorithm. Right figure: there is a basin that is a set-wise strict local-min.

Kawaguchi [131], Laurent and Brecht [108], Nouiehed and Razaviyayn [152], Zhang [233] proved the result under relaxed conditions or provided simpler proofs. Yun et al. [227] and Zou et al. [239] present necessary and sufficient conditions for a stationary point to be a global minimum.

Deep over-parameterized networks. Over-parameterized networks are the simplest non-linear networks that currently can be analyzed, but already somewhat subtle. It is widely believed that "more parameters than necessary" can smooth the landscape [128, 148, 230], but these works do not provide a rigorous result. To obtain rigorous results, one common assumption for deep networks is that the last layer has more neurons than the number of samples. Under this assumption on the width of the last layer, Nguyen et al. [151] and Li et al. [115] prove that a fully connected network has no "spurious valley" or "set-wise strict local minima", for generic input data. Intuitively, "set-wise strict local minima" and "spurious valley" are the "bad basin" illustrated in the right figure of Figure 3 (see [151] or [115] for formal definitions).

The above works can be viewed as the extensions of a classical work [225] on 1-hidden-layer over-parameterized networks (with sigmoid activations), which claimed to have proved that every local-min is a global-min. It was pointed out that the proof is not rigorous, and a counter-example was constructed [115, 50]. Ding et al. [50] further constructs sub-optimal local-min for arbitrarily wide neural networks for a large class of activations including sigmoid activations, thus under the settings of [225][151] [115] sub-optimal local minima can exist. This implies that overparameterization cannot eliminate bad local minima, but only eliminate bad basins (or spurious valleys) without extra assumptions or modifications.

Intuitively, over-parameterized networks are prone to over-fitting, but many practical networks are indeed over-parameterized and understanding why over-fitting does not happen is an interesting line of research [148, 18, 209, 213, 21, 138]. In this article, we mainly discuss the research on the optimization side.

Modified problems. The results discussed so far mainly study the original neural network problem (3), and the landscape is different if the problem is slightly changed. Liang et al. [121] considered modified neuron activation and an extra regularizer for an arbitrary deep neural-net, for binary classification problems, and prove that no bad local-min exists. Kawaguchi et al. [100] extends the result of [121] to multi-class classification problems. In addition, [100] provides toy examples to illustrate the limitation of only considering local minima: GD may diverge for the modified problem. It is a possible weakness of any result on "no bad local-min" including the classical works on deep linear networks. In fact, as discussed in Section 3.2, the possibility of divergence (U2) is one of the two undesirable situations that classical results on GD does not exclude, and eliminating bad local-min does not rule out the possibility of (U2). Liang et al. [123] showed that for a deep CNN with certain activation function, adding a regularizer can ensure there is no sub-optimal local-min and no decreasing path to infinity, thus eliminating (U2).

Negative results. Most of the works in GON area after 2012 are positive results. However, while neural-nets can be trained in some cases with careful choices of architecture, initial points and parameters, there are still many cases that neural-nets cannot be successfully trained. Shalev et al. [179] explained a few possible reasons of failure of GD for training neural networks. There are a number of recent works focusing the existence of bad local minima (here "bad" means "sub-optimal").

These negative results differ by their assumptions on activation functions, data distribution and network structure. As for the activation functions, many works showed that ReLU networks have bad local minima (e.g., Swirszcz et al.[192] Zhou et al. [238], Safran et al.[172], Venturi et al.[205], Liang et al.[122]), and a few works Liang et al. [122], Yun et al.[228] and Ding et al. [50] construct examples for smooth activations. As for the loss function, Safran and Shamir [172] and Venturi et al. [205] analyze the population risk (expected loss) and other works analyze the empirical risk (finite sum loss). As for the data distribution, most works consider data points that lie in a zero-measure space or satisfy special requirements like linear separability (Liang et al. [122]) and Gaussian (Safran et al.[172]), and few works consider generic input data (e.g. Ding et al. [50]). We refer the readers to Ding et al. [50] which compared various examples of bad local-min in a table.

6.3.2 Algorithmic analysis of deep networks

A good landscape may explain the nice properties of the optimization formulation, but does not fully explain the behavior of specific algorithms. To understand specific algorithms, convergence analysis is more desirable. However, for a general neural-net the convergence analysis is extremely difficult, thus some assumptions have to be made. The current local (algorithmic) analysis of deep neural-nets is mainly performed for two types: linear networks [175, 17, 9, 95] and ultra-wide networks.

Linear networks. Arora et al. [9] considered the problem $\min_{W_1,\dots,W_L} \|W_1 W_2 \dots W_L - \Phi\|_F^2$, and prove that if the initial weights are "balanced" and the initial product $W_1 \dots W_L$ is close to Φ, GD with a small stepsize converges to global minima in polynomial time. Ji and Telgarsky [95] assume linearly separable data and prove that if the initial objective value is less than a certain threshold, then GD with small adaptive stepsize converges asymptotically to global minima.

Neural Tangent Kernel (NTK) and linearization. Consider the neural-network problem with quadratic loss $\min_\theta \sum_{i=1}^n \frac{1}{2}(f_\theta(x_i) - y_i)^2$, where $x_i \in \mathbb{R}^d, y_i \in \mathbb{R}$ (it can be generalized to multi-dimensional output and non-quadratic loss). The gradient descent dynamics is

$$\frac{d\theta}{dt} = -\sum_i \frac{\partial f_\theta(x_i)}{\partial \theta}(f_\theta(x_i) - y_i). \tag{24}$$

Define $G = (\frac{\partial f_\theta(x_1)}{\partial \theta}, \ldots, \frac{\partial f_\theta(x_n)}{\partial \theta}) \in \mathbb{R}^{P \times n}$ where P is the number of parameters, and define *neural tangent kernel* $K = G^T G$. Let $r = (f_\theta(x_1) - y_1; \ldots; f_\theta(x_n) - y_n)$, then $\frac{dr_i}{dt} = \frac{\partial f_\theta(x_i)}{\partial \theta} \sum_j \frac{\partial f_\theta(x_j)}{\partial \theta} r_j$, or equivalently,

$$\frac{dr}{dt} = -K(t)r, \tag{25}$$

When $f_\theta(x) = \theta^T x$, the matrix $K(t)$ reduces to a constant matrix $X^T X$, thus (25) reduces to $\frac{dr(t)}{dt} = -X^T X r(t)$.

Jacot et al. [91] proved that $K(t)$ is a constant matrix for any t under certain conditions. More specifically, if the initial weights are i.i.d. Gaussian with certain variance, then as the number of neurons at each layer goes to infinity sequentially, $K(t)$ converges to a constant matrix K_c (uniformly for all $t \in [0, T]$ where T is a given constant). Under further assumptions on the activations (non-polynomial activations) and data (distinct data from the unit sphere), [91] proves that K_c is positive definite. One interesting part of [91] is that the limiting NTK matrix K_c has a closed form expression, computed recursively by an analytical formula. Du et al. [56] has also analyzed the same kernel for an ultra-wide neural networks.

Yang [220] and Novak et al. [153] extended [91]: they only require the width of each layer goes to infinitely simultaneuously (instead of sequentially in [91]), and provides a formula of NTK for convolutional networks, called CNTK.

Finite-width Ultra-wide networks. Around the same time as [91], Allen-Zhu et al. [4] and Zou et al. [241] and Du et al. [56] analyzed deep ultra-wide non-linear networks and prove that with Gaussian initialization and small enough step-size, GD and/or SGD converge to global minima (these works can be viewed extensions of an analysis of a 1-hidden-layer networks [118, 56]). In contrast to the landscape results [115, 151] that only require one layer to have n neurons, these works require a much larger number of neurons per layer: $O(n^{24}L^{12}/\delta^8)$ in [4] where $\delta = \min_{i \neq j} \|x_i - x_j\|$ and $O(n^4/\lambda_{\min}(K)^4)$ in [56] where K is a complicated matrix defined recursively. Arora et al. [10] also analyzed finite-width networks, by proving a non-asymptotic version of the NTK result of [91]. Zhang et al. [232], Ma et al. [134] analyzed the convergence of over-parameterized ResNet.

NTK as a computation tool. The explicit formula of the limiting NTK makes it possible to actually compute NTK and perform kernel gradient descent for a real-world problem, which provides an alternative to standard neural-nets. As computing the CNTK directly is time consuming, Novak et al. [153] used Monte Carlo sampling to approximately compute CNTK. Arora et al. [10] proposed an exact efficient algorithm to compute CNTK and tests it on CIFAR10, achieving 77% test accuracy for CNTK with global average pooling. Li et al. [120] utilized two further tricks to achieve 89% test accuracy on CIFAR10, on par with AlexNet. Arora et al. [11] showed that NTK can perform better than standard neural-nets on small-scale datasets. Novak et al. [154] built a python library called "neural tangents" that makes NTK more accessible. These works showed that a theoretically-derived tool can lead to computational advances, at least in certain tasks.

Linearized networks as a computation tool. Another computational tool suggested by NTK is to directly use the linearized network $f_{\text{lin}}(\theta) = f(\theta_0) + \langle \theta, \nabla f(\theta_0) \rangle$ as a replacement of the original neural-net. Even if the width is finite, one could always use such a linearized neural-net to perform computation. An immediate question is whether this linearized network performs well in practice. Lee et al. [112] showed that a linearized network can achieve somewhat similar performance as a standard neural-net when using a quadratic loss, thus providing partial validation to this approach. More study is needed to understand whether linearized networks can be practically useful in certain cases.

Mean-field approximation: another group of works. There are another group of works which also studied infinite-width limit of SGD. Sirignano and Spiliopoulos [182] considered discrete-time SGD for infinite-width multi-layer neural networks, and showed that the limit of the neural network output satisfies a certain differential equation. Araujo et al. [8], Nguyen [149] also studied infinite-width multi-layer networks. These works are extensions of previous works Mei et al. [139], Srignanao and Spiliopoulos [181] and Rotskoff and Vanden-Eijnden [170], which analyzed 1-hidden-layer networks. A major difference between these works and [91] [4] [241] [56] is the scaling factor; for instance, Sirignano and Spiliopoulos [181] considered the scaling factor 1/fan-in, while [91] [4] [241] [56] considered the scaling factor $1/\sqrt{\text{fan-in}}$. The latter scaling factor of $1/\sqrt{\text{fan-in}}$ is used in Bottou initialization (corresponding to variance 1/fan-in), thus closer to practice, but they imply that the parameters move very little as the number of parameters increase. In contrast, [139, 181, 170, 182, 8, 149] show that the parameters evolve according to a PDE and thus can move far away from the initial point.

"Lazy training" and two learning schemes. The high-level idea of [91] [4] [241] [56] is termed "lazy training" by [40]: the model behaves like its linearization around its initial point. Because of the huge number of parameters, each parameter only needs to move a tiny amount, thus linearization is a good approximation. However, practical networks are not ultra-wide, thus the parameters will move a reasonably large amount of distance, and likely to move out of the linearization regimes. [40] indeed showed that the behavior of SGD in practical neural-nets is different from lazy training. Note that [112] made an opposite claim that wide neural-nets behave similarly to its linearization. We suspect that this difference is because [112] is using a quadratic loss for a classification problem, while [40] uses the standard cross-entropy loss for the classification problem. [40] also pointed out that "lazy training" is mainly due to implicit choice of the scaling factor, and applies to a large class of models beyond neural networks. A natural question is whether the "adaptive learning scheme" described by [139, 181, 170, 182, 8, 149] can partially characterize the behavior of SGD. In an effort to answer this question, Williams et al. [210] analyzed a 1-hidden-layer ReLU network with 1-dimensional input, and provided conditions for the "kernel learning scheme" and "adaptive learning scheme".

6.4 Research in Shallow Networks after 2012

For the ease of presentation, results for shallow networks are mainly reviewed in this subsection. Due to the large amount of literature in GON area, it is hard to review all recent works, and we can only give an incomplete overview. We group these works based on the following criteria: landscape or algorithmic analysis (first-level classification criterion); one-neuron, 2-layer network or 1-hidden-layer network [13] (second-level criterion). Note that among the works in the same class, they may differ on the assumption on input data (Gaussian input and linearly separable input are common), number of neurons, loss function and specific algorithms (GD, SGD or others). This section focuses on positive results, and negative results for shallow networks are discussed in Section 6.3.1.

Global landscape of 1-hidden-layer neural-nets. There have been many works on the landscape of 1-hidden-layer neural-nets. One interesting work (mentioned earlier when discussing mode connectivity) is Freeman and Bruna [65] which proved that the sub-level set is connected for deep linear networks and 1-hidden-layer ultra-wide ReLU networks. This does not imply every local-min is global-min, but implies there is no spurious valley (and no bad strict local-min). A related recent work is Venturi et al. [204] which proved no spurious valley exists (implying no bad basin) for 1-hidden-layer network with "low intrinsic dimension". Haeffele and Vidal [80] extended the classical work of Burer and Monteiro [33] to 1-hidden-layer neural-net, and proved that a subset of the local minima are global minima, for a set of positive homogeneous activations. Ge et al. [68] and Gao et al. [66] designed a new loss function so that all local minima are global minima. Feizi et al. [60] designed a special network for which almost all local minima are global minima. Panigrahy et al. [161] analyzed local minima for many special neurons via electrodynamics theory. For quadratic activations, Soltanolkotabi et al. [187] proved that 2-layer over-parameterized network with width no less than $O(\sqrt{n})$ have no bad local-min for almost all input data, and Liang et al. [122] provided a sufficient and necessary condition for the data distribution so that 1-hidden-layer neural-net has no bad local-min (no matter what the width is). For 1-hidden-layer ReLU networks (without bias term), Soudry and Hoffer [188] proved that the number of differentiable local minima is very small. Nevertheless, Laurent and von Brecht [109] showed that except flat bad local minima, all local minima of 1-hidden-layer ReLU networks (with bias term) are non-differentiable. Liang et al. [122] proved that for linearly separable data, a 1-hidden-layer net with smooth strictly increasing neurons has no bad local-min.

Algorithmic analysis of 2-layer neural-nets. There are many works on the algorithmic analysis of SGD for shallow networks under a variety of settings. The first class analyzed SGD for 2-layer neural-networks (with the second layer weights fixed). A few works mainly analyzed one single neuron. Tian [197] and Soltanolkotabi [187] analyzed the performance of GD for a single ReLU neuron. Mei et al. [139] analyzed a single sigmoid neuron. Other works analyzed 2-layer networks with multiple neurons. Brutzkus and Globerson [32] analyzed a non-overlapping 2-layer ReLU network and proved that the problem is NP-complete for general input, but if the

[13] In this section, we will use "2-layer network" to denote a network like $y = \phi(Wx + b)$ or $y = V^*\phi(Wx + b)$ with fixed V^*, and use "1-hidden-layer network" to denote a network like $y = V\phi(Wx + b_1) + b_2$ with both V and W being variables.

input is Gaussian then GD converges to global minima in polynomial time. Zhong et al. [235] analyzed 2-layer under-parameterized network (no more than d neurons) for Gaussian input and initialization by tensor method. Li et al. [119] analyzed 2-layer network with skip connection for Gaussian input. Brutzkus et al. [31] analyzed 2-layer over-parameterized network with leaky ReLU activation for linearly seperable data. Wang et al. [207] and Zhang et al. [234] analyzed 2-layer over-parameterized network with ReLU activation, for linearly separable input and Gaussian input respectively. Du et al. [54] analyzed 2-layer over-parameterized network with quadratic neuron for Gaussian input. Oymak and Soltanolkotabi [160] proved the global convergence of GD with random initialization for a 2-layer network with a few types of neuron activations, when the number of parameters exceed $O(n^2)$ ($O(\cdot)$ here hides condition number and other parameters). Su and Yang [191] analyzed GD for 2-layer ReLU network with $O(n)$ neurons for generic input data.

Algorithmic analysis of 1-hidden-layer neural-nets. The second class analyzed 1-hidden-layer neural-network (with the second layer weights trainable). The relation of 1-hidden-layer network and tensors is explored in [94, 144]. Boob and Lan [26] analyzed a specially designed alternating minimization method for over-parameterized 1-hidden-layer neural-net. Du et al. [55] analyzed an non-overlapping network for Gaussian input and with an extra normalization, and proved that SGD can converge to global-min for some initialization and converge to bad local-min for other initialization. Vempala and Wilmes [203] proved that for random initialization and with $n^{O(k)}$ neurons, GD converges to the best degree k polynomial approximation of the target function; a matching lower bound is also proved. Ge et al. [69] analyzed a new spectral method for learning 1-hidden-layer network. Oymak and Soltanolkotabi [159] analyzed GD for a rather general problem and applied it to 1-hidden-layer neural-net where $n \leq d$ (number of samples no more than dimension) for any number of neurons.

7 Concluding Remarks

In this article, we have reviewed existing theoretical results related to neural network optimization, mainly focusing on the training of feedforward neural networks. The goal of theory in general is two-fold: understanding and design. As for understanding, now we have a good understanding on the effect of initialization on stable training, and some understanding on the effect of over-parameterization on the landscape. As for design, theory has already greatly helped the design of algorithms (e.g. initialization schemes, batch normalization, Adam). There are also examples like CNTK that is motivated from theoretical analysis and has become a real tool. Besides design and understanding, some interesting empirical phenomenons have been discovered, such as mode connectivity and lottery ticket hypothesis, awaiting more theoretical studies. Overall, there is quite some progress in the theory for neural-net optimization.

That being said, there are still lots of challenges. We still do not understand many of the components that affect the practical performance of neural networks, e.g., the neural architecture and Adam optimizer. As a result, there are many problems beyond image classification that cannot be solved well by neural networks, yet it is unclear whether the optimization part has been done properly. Bringing theory closer to practice is still a huge challenge for both theoretical and empirical researchers. One of the biggest doubts on this area may be how far the theory can go. Have we already hit the glass ceiling that theory can barely provide more guidance? It is hard to say, and more time is needed. In the history of linear programming, after the invention of simplex method in 1950's, for 20 years it is also not clear whether a polynomial time algorithm exists for solving LP, until the ellipsoid method was proposed; and it took another 10 years for a method that is both practical and theoretically strong (interior point method) to appear. Maybe it just takes another decade or more decades to see a rather complete theory for neural network optimization.

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A Review of Large-scale (Convex) Optimization Methods

In this subsection, we review several methods in large-scale optimization that are closely related to deep learning.

Since the neural network optimization problem is often of huge size (at least millions of optimization variables and millions of samples), a method that directly inverts a matrix in an iteration, such as Newton method, is often considered impractical. Thus we will focus on first-order methods, i.e., iterative algorithms that mainly use gradient information (though we will briefly discuss quasi-Newton methods).

To unify these methods in one framework, we start with the common convergence rate results of gradient descent method (GD) and explain how different methods improve the convergence rate in different ways. Consider the prototype convergence rate result in convex optimization: the epoch-complexity [14] is $O(\kappa \log 1/\epsilon)$ or $O(\beta/\epsilon)$. These rates mean the following: to achieve ϵ error, the number of epochs to achieve error ϵ is no more than $\kappa \log 1/\epsilon$ for strongly convex problems (or β/ϵ for convex problems), where κ is the condition number of the problem (and β is the maximal Lipschitz constant of all gradients).

There are at least four classes of methods that can improve the convergence rate $O(\kappa \log 1/\epsilon)$

[14] For batch GD, one epoch is one iteration. For SGD, one epoch consists of multiple stochastic gradient steps that pass all data points once. We do not say "iteration complexity" or "the number of iterations" since per-iteration cost for the vanilla gradient descent and SGD are different and can easily cause confusion. In contrast, the per-epoch cost (number of operations) for batch GD and SGD are comparable.

for strongly convex quadratic problems [15].

The first class of methods are based on decomposition, i.e. decomposing a large problem into smaller ones. Typical methods including SGD and coordinate descent (CD). The theoretical benefit is relatively well understood for CD, and somewhat well understood for SGD type methods. A simple argument of the benefit [30] is the following: if all training samples are the same, then the gradient for one sample is proportional to the gradient for all samples, thus one iteration of SGD gives the same update as one iteration of GD; since one iteration of GD takes n-times more computation cost than one iteration of SGD, thus GD is n times slower than SGD. Below we discuss more precise convergence rate results that illustrate the benefit of CD and SGD. For an unconstrained n-dimensional convex quadratic problem with all diagonal entries being 1 [16]:

- Randomized CD has an epoch-complexity $O(\kappa_{CD} \log 1/\epsilon)$ [114, 146], where κ_{CD} is the ratio of the average eigenvalue λ_{avg} over the minimum eigenvalue $\lambda_{\min}$ of the coefficient matrix. This is smaller than $O(\kappa_{CD} \log 1/\epsilon)$ by a factor of $\lambda_{\max}/\lambda_{\text{avg}}$ where $\lambda_{\max}$ is the maximum eigenvalue. Clearly, the improvement ratio $\lambda_{\max}/\lambda_{\text{avg}}$ lies in $[1, n]$, thus randomized CD is 1 to n times faster than GD.

- For SGD type methods, very similar acceleration can be proved. Recent variants of SGD (such as SVRG [97] and SAGA [46]) achieve the same convergence rate as R-CD for the equal-diagonal quadratic problems (though not pointed out in the literature), and are also 1 to n times faster than GD. We highlight that this up-to-n-factor acceleration has been the major focus of recent studies of SGD type methods, and has achieved much attention in theoretical machine learning area.

- Classical theory of vanilla SGD [30] often uses diminishing stepsize and thus does not enjoy the same benefit as SVRG and SAGA; however, as mentioned before, constant step-size SGD works quite well in many machine learning problems, and in these problems SGD may have inherited the same advantage of SVRG and SAGA.

The second class of methods are fast gradient methods (FGM) that have convergence rate $O(\sqrt{\kappa} \log 1/\epsilon)$, thus saving a factor of $\sqrt{\kappa}$ compared to the convergence rate of GD $O(\kappa \log 1/\epsilon)$. FGM includes conjugate gradient method, heavy ball method and accelerated gradient method. For quadratic problems, these three methods all achieve the improved rate $O(\sqrt{\kappa} \log 1/\epsilon)$. For general strongly convex problems, only accelerated gradient method is known to achieve the rate $O(\sqrt{\kappa} \log 1/\epsilon)$.

The third class of methods utilize the second order information of the problem, including quasi-Newton method and Barzilai-Borwein method. Quasi-Newton methods such as BFGS and limited BFGS (see, e.g., [212]) use an approximation of the Hessian in each epoch, and are popular choices

[15] Note that the methods discussed below also improve the rate for convex problems but we skip the discussions

[16] The results for general convex problems are also established, but we discuss a simple case for the ease of presentation. Here we assume the dimension and the number of samples are both n, and a refined analysis can show the dependence on the two parameters.

for many nonlinear optimization problems. Barzilai-Borwein (BB) method uses a diagonal matrix estimation of the Hessian, and can also be viewed as GD with a special stepsize that approximates the curvature of the problem. It seems very difficult to theoretically justify the advantage of these methods over GD, but intuitively, the convergence speed of these methods rely much less on the condition number κ (or any variant of the condition number such as κ_{CD}). A rigorous time complexity analysis of any method in this class, even for unconstrained quadratic problems, remains largely open.

The fourth class of methods are parallel computation methods, which can be combined with aforementioned three classes of ingredients. As discussed in the classical book [24], GD is a special case of Jacobi method which is naturally parallelizable, and CD is a Gauss-Seidel type method which may require some extra trick to parallize. For example, for minimizing a n-dimensional least square problem, each epoch of GD mainly requires a matrix-vector product which is parallelizable. More specifically, while a serial model takes $O(n^2)$ time steps to perform a matrix-vector product, a parallel model can take as small as $O(\log n)$ operations. For CD or SGD, each iteration consists of one or a few vector-vector products, and each vector-vector product is parallelizable. Multiple iterations in one epoch of CD or SGD may not be parallellizable in the worst case (e.g. a dense coefficient matrix), but when the problem exhibits some sparsity (e.g. the coefficient matrix is sparse), they can be partially parallelizable. The above discussion seems to show that "batch" methods such as GD might be faster than CD or SGD in a parallel setting; however, it is an over-simplified discussion, and many other factors such as synchronization cost and the communication burden can greatly affect the performance. In general, parallel computation in numerical optimization is quite complicated, which is why the whole book [24] is devoted to this topic.

We briefly summarize the benefits of these methods as below. For minimizing n-dimensional quadratic functions (with equal diagonal entries), the benchmark GD takes time $O(n^2 \kappa \log 1/\epsilon)$ to achieve error ϵ. The first class (e.g. accelerated gradient method) improves it to $O(n^2 \sqrt{\kappa} \log 1/\epsilon)$, the second class (e.g. CD and SVRG) improves it to $O(n^2 \kappa_{CD} \log 1/\epsilon)$, the third class (e.g. BFGS and BB) may improve κ to some other unknown parameter, and the fourth class (parallel computation) can potentially improve it to $O(\kappa \log n \log 1/\epsilon)$ with extra cost such as communication. Although we treat these methods as separate classes, researchers have extensively studied various mixed methods of two or more classes, though the theoretical analysis can be much harder. Even just for quadratic problems, the theoretical analysis cannot fully predict the practical behavior of these algorithms or their mixtures, but these results provide quite useful understanding. For general convex and non-convex problems, some part of the above theoretical analysis can still hold, but there are still many unknown questions.

References

[1] Takuya Akiba, Shuji Suzuki, and Keisuke Fukuda. Extremely large minibatch sgd: training resnet-50 on imagenet in 15 minutes. *arXiv preprint arXiv:1711.04325*, 2017.

[2] Zeyuan Allen-Zhu. Katyusha: The first direct acceleration of stochastic gradient methods. *The Journal of Machine Learning Research*, 18(1):8194–8244, 2017.

[3] Zeyuan Allen-Zhu. Natasha 2: Faster non-convex optimization than sgd. In *Advances in Neural Information Processing Systems*, pages 2680–2691, 2018.

[4] Zeyuan Allen-Zhu, Yuanzhi Li, and Zhao Song. A convergence theory for deep learning via over-parameterization. *arXiv preprint arXiv:1811.03962*, 2018.

[5] Shun-ichi Amari and Hiroshi Nagaoka. *Methods of information geometry*, volume 191. American Mathematical Soc., 2007.

[6] Shun-Ichi Amari, Hyeyoung Park, and Kenji Fukumizu. Adaptive method of realizing natural gradient learning for multilayer perceptrons. *Neural Computation*, 12(6):1399–1409, 2000.

[7] Rohan Anil, Vineet Gupta, Tomer Koren, Kevin Regan, and Yoram Singer. Second order optimization made practical. *arXiv preprint arXiv:2002.09018*, 2020.

[8] Dyego Araujo, Roberto I. Oliveira, and Daniel Yukimura. A mean-field limit for certain deep neural networks, 2019.

[9] Sanjeev Arora, Nadav Cohen, Noah Golowich, and Wei Hu. A convergence analysis of gradient descent for deep linear neural networks. *arXiv preprint arXiv:1810.02281*, 2018.

[10] Sanjeev Arora, Simon S Du, Wei Hu, Zhiyuan Li, Ruslan Salakhutdinov, and Ruosong Wang. On exact computation with an infinitely wide neural net. *arXiv preprint arXiv:1904.11955*, 2019.

[11] Sanjeev Arora, Simon S Du, Zhiyuan Li, Ruslan Salakhutdinov, Ruosong Wang, and Dingli Yu. Harnessing the power of infinitely wide deep nets on small-data tasks. *arXiv preprint arXiv:1910.01663*, 2019.

[12] Sanjeev Arora, Zhiyuan Li, and Kaifeng Lyu. Theoretical analysis of auto rate-tuning by batch normalization. In *International Conference on Learning Representations*, 2019. URL `https://openreview.net/forum?id=rkxQ-nA9FX`.

[13] Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. Layer normalization. *arXiv preprint arXiv:1607.06450*, 2016.

[14] Marco Baity-Jesi, Levent Sagun, Mario Geiger, Stefano Spigler, G Ben Arous, Chiara Cammarota, Yann LeCun, Matthieu Wyart, and Giulio Biroli. Comparing dynamics: Deep neural networks versus glassy systems. *arXiv preprint arXiv:1803.06969*, 2018.

[15] David Balduzzi, Marcus Frean, Lennox Leary, JP Lewis, Kurt Wan-Duo Ma, and Brian McWilliams. The shattered gradients problem: If resnets are the answer, then what is the question? In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 342–350. JMLR. org, 2017.

[16] Anas Barakat and Pascal Bianchi. Convergence analysis of a momentum algorithm with adaptive step size for non convex optimization. *arXiv preprint arXiv:1911.07596*, 2019.

[17] Peter Bartlett, Dave Helmbold, and Phil Long. Gradient descent with identity initialization efficiently learns positive definite linear transformations. In *International Conference on Machine Learning*, pages 520–529, 2018.

[18] Peter L Bartlett, Dylan J Foster, and Matus J Telgarsky. Spectrally-normalized margin bounds for neural networks. In *Advances in Neural Information Processing Systems*, pages 6240–6249, 2017.

[19] Jonathan Barzilai and Jonathan M Borwein. Two-point step size gradient methods. *IMA journal of numerical analysis*, 8(1):141–148, 1988.

[20] Sue Becker, Yann Le Cun, et al. Improving the convergence of back-propagation learning with second order methods. In *Proceedings of the 1988 connectionist models summer school*, pages 29–37, 1988.

[21] Mikhail Belkin, Daniel Hsu, Siyuan Ma, and Soumik Mandal. Reconciling modern machine learning and the bias-variance trade-off. *arXiv preprint arXiv:1812.11118*, 2018.

[22] Albert S Berahas, Majid Jahani, and Martin Takáč. Quasi-newton methods for deep learning: Forget the past, just sample. *arXiv preprint arXiv:1901.09997*, 2019.

[23] Dimitri P Bertsekas. Nonlinear programming. *Journal of the Operational Research Society*, 48(3): 334–334, 1997.

[24] Dimitri P Bertsekas and John N Tsitsiklis. *Parallel and distributed computation: numerical methods*, volume 23. Prentice hall Englewood Cliffs, NJ, 1989.

[25] Nils Bjorck, Carla P Gomes, Bart Selman, and Kilian Q Weinberger. Understanding batch normalization. In *Advances in Neural Information Processing Systems*, pages 7694–7705, 2018.

[26] Digvijay Boob and Guanghui Lan. Theoretical properties of the global optimizer of two layer neural network. *arXiv preprint arXiv:1710.11241*, 2017.

[27] Antoine Bordes, Léon Bottou, and Patrick Gallinari. Sgd-qn: Careful quasi-newton stochastic gradient descent. *Journal of Machine Learning Research*, 10(Jul):1737–1754, 2009.

[28] Léon Bottou. Reconnaissance de la parole par reseaux connexionnistes. In *Proceedings of Neuro Nimes 88*, pages 197–218, Nimes, France, 1988. URL `http://leon.bottou.org/papers/bottou-88b`.

[29] Léon Bottou. Online learning and stochastic approximations. *On-line learning in neural networks*, 17 (9):142, 1998.

[30] Léon Bottou, Frank E Curtis, and Jorge Nocedal. Optimization methods for large-scale machine learning. *SIAM Review*, 60(2):223–311, 2018.

[31] A. Brutzkus, A. Globerson, E. Malach, and S. Shalev-Shwartz. Sgd learns over-parameterized networks that provably generalize on linearly separable data. *ICLR*, 2018.

[32] Alon Brutzkus and Amir Globerson. Globally optimal gradient descent for a convnet with gaussian inputs. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 605–614. JMLR. org, 2017.

[33] Samuel Burer and Renato DC Monteiro. Local minima and convergence in low-rank semidefinite programming. *Mathematical Programming*, 103(3):427–444, 2005.

[34] Yongqiang Cai, Qianxiao Li, and Zuowei Shen. A quantitative analysis of the effect of batch normalization on gradient descent. In *International Conference on Machine Learning*, pages 882–890, 2019.

[35] Yair Carmon, John C Duchi, Oliver Hinder, and Aaron Sidford. Convex until proven guilty: Dimension-free acceleration of gradient descent on non-convex functions. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 654–663. JMLR. org, 2017.

[36] Yair Carmon, John C Duchi, Oliver Hinder, and Aaron Sidford. Accelerated methods for nonconvex optimization. *SIAM Journal on Optimization*, 28(2):1751–1772, 2018.

[37] Pratik Chaudhari, Anna Choromanska, Stefano Soatto, Yann LeCun, Carlo Baldassi, Christian Borgs, Jennifer Chayes, Levent Sagun, and Riccardo Zecchina. Entropy-sgd: Biasing gradient descent into wide valleys. *arXiv preprint arXiv:1611.01838*, 2016.

[38] Xiangyi Chen, Sijia Liu, Ruoyu Sun, and Mingyi Hong. On the convergence of a class of adam-type algorithms for non-convex optimization. *arXiv preprint arXiv:1808.02941*, 2018.

[39] Yuejie Chi, Yue M Lu, and Yuxin Chen. Nonconvex optimization meets low-rank matrix factorization: An overview. *IEEE Transactions on Signal Processing*, 67(20):5239–5269, 2019.

[40] Lenaic Chizat, Edouard Oyallon, and Francis Bach. On lazy training in differentiable programming, 2018.

[41] Frank E Curtis and Katya Scheinberg. Optimization methods for supervised machine learning: From linear models to deep learning. In *Leading Developments from INFORMS Communities*, pages 89–114. INFORMS, 2017.

[42] Yann N Dauphin and Samuel Schoenholz. Metainit: Initializing learning by learning to initialize. In *Advances in Neural Information Processing Systems*, pages 12624–12636, 2019.

[43] Yann N Dauphin, Razvan Pascanu, Caglar Gulcehre, Kyunghyun Cho, Surya Ganguli, and Yoshua Bengio. Identifying and attacking the saddle point problem in high-dimensional non-convex optimization. In *Advances in neural information processing systems*, pages 2933–2941, 2014.

[44] Soham De, Anirbit Mukherjee, and Enayat Ullah. Convergence guarantees for rmsprop and adam in non-convex optimization and an empirical comparison to nesterov acceleration. 2018.

[45] Aaron Defazio and Léon Bottou. On the ineffectiveness of variance reduced optimization for deep learning. In *Advances in Neural Information Processing Systems*, pages 1753–1763, 2019.

[46] Aaron Defazio, Francis Bach, and Simon Lacoste-Julien. Saga: A fast incremental gradient method with support for non-strongly convex composite objectives. In *Advances in neural information processing systems*, pages 1646–1654, 2014.

[47] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv preprint arXiv:1810.04805*, 2018.

[48] Olivier Devolder, François Glineur, Yurii Nesterov, et al. First-order methods with inexact oracle: the strongly convex case. *CORE Discussion Papers*, 2013016, 2013.

[49] Olivier Devolder, François Glineur, and Yurii Nesterov. First-order methods of smooth convex optimization with inexact oracle. *Mathematical Programming*, 146(1-2):37–75, 2014.

[50] Tian Ding, Dawei Li, and Ruoyu Sun. Spurious local minima exist for almost all over-parameterized neural networks. *optimization online*, 2019.

[51] Laurent Dinh, Razvan Pascanu, Samy Bengio, and Yoshua Bengio. Sharp minima can generalize for deep nets. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 1019–1028. JMLR. org, 2017.

[52] Timothy Dozat. Incorporating nesterov momentum into adam. 2016.

[53] Felix Draxler, Kambis Veschgini, Manfred Salmhofer, and Fred A Hamprecht. Essentially no barriers in neural network energy landscape. *arXiv preprint arXiv:1803.00885*, 2018.

[54] Simon S Du and Jason D Lee. On the power of over-parametrization in neural networks with quadratic activation. *arXiv preprint arXiv:1803.01206*, 2018.

[55] Simon S Du, Jason D Lee, Yuandong Tian, Barnabas Poczos, and Aarti Singh. Gradient descent learns one-hidden-layer cnn: Don't be afraid of spurious local minima. *arXiv preprint arXiv:1712.00779*, 2017.

[56] Simon S Du, Jason D Lee, Haochuan Li, Liwei Wang, and Xiyu Zhai. Gradient descent finds global minima of deep neural networks. *arXiv preprint arXiv:1811.03804*, 2018.

[57] John Duchi, Elad Hazan, and Yoram Singer. Adaptive subgradient methods for online learning and stochastic optimization. *Journal of Machine Learning Research*, 12(Jul):2121–2159, 2011.

[58] Dumitru Erhan, Yoshua Bengio, Aaron Courville, Pierre-Antoine Manzagol, Pascal Vincent, and Samy Bengio. Why does unsupervised pre-training help deep learning? *Journal of Machine Learning Research*, 11(Feb):625–660, 2010.

[59] Cong Fang, Chris Junchi Li, Zhouchen Lin, and Tong Zhang. Spider: Near-optimal non-convex optimization via stochastic path-integrated differential estimator. In *Advances in Neural Information Processing Systems*, pages 687–697, 2018.

[60] Soheil Feizi, Hamid Javadi, Jesse Zhang, and David Tse. Porcupine neural networks:(almost) all local optima are global. *arXiv preprint arXiv:1710.02196*, 2017.

[61] O. P. Ferreira and S. Z. Németh. On the spherical convexity of quadratic functions. *Journal of Global Optimization*, 73(3):537–545, Mar 2019. ISSN 1573-2916. doi: 10.1007/s10898-018-0710-6. URL `https://doi.org/10.1007/s10898-018-0710-6`.

[62] Jonathan Frankle and Michael Carbin. The lottery ticket hypothesis: Finding sparse, trainable neural networks. *arXiv preprint arXiv:1803.03635*, 2018.

[63] Jonathan Frankle, Gintare Karolina Dziugaite, Daniel M Roy, and Michael Carbin. The lottery ticket hypothesis at scale. *arXiv preprint arXiv:1903.01611*, 2019.

[64] Silvio Franz, Sungmin Hwang, and Pierfrancesco Urbani. Jamming in multilayer supervised learning models. *arXiv preprint arXiv:1809.09945*, 2018.

[65] C Daniel Freeman and Joan Bruna. Topology and geometry of half-rectified network optimization. *arXiv preprint arXiv:1611.01540*, 2016.

[66] Weihao Gao, Ashok Vardhan Makkuva, Sewoong Oh, and Pramod Viswanath. Learning one-hidden-layer neural networks under general input distributions. *arXiv preprint arXiv:1810.04133*, 2018.

[67] Timur Garipov, Pavel Izmailov, Dmitrii Podoprikhin, Dmitry P Vetrov, and Andrew G Wilson. Loss surfaces, mode connectivity, and fast ensembling of dnns. In *Advances in Neural Information Processing Systems*, pages 8789–8798, 2018.

[68] Rong Ge, Jason D Lee, and Tengyu Ma. Learning one-hidden-layer neural networks with landscape design. *arXiv preprint arXiv:1711.00501*, 2017.

[69] Rong Ge, Rohith Kuditipudi, Zhize Li, and Xiang Wang. Learning two-layer neural networks with symmetric inputs. *arXiv preprint arXiv:1810.06793*, 2018.

[70] Mario Geiger, Stefano Spigler, Stéphane d'Ascoli, Levent Sagun, Marco Baity-Jesi, Giulio Biroli, and Matthieu Wyart. The jamming transition as a paradigm to understand the loss landscape of deep neural networks. *arXiv preprint arXiv:1809.09349*, 2018.

[71] Behrooz Ghorbani, Shankar Krishnan, and Ying Xiao. An investigation into neural net optimization via hessian eigenvalue density. *arXiv preprint arXiv:1901.10159*, 2019.

[72] Dar Gilboa, Bo Chang, Minmin Chen, Greg Yang, Samuel S Schoenholz, Ed H Chi, and Jeffrey Pennington. Dynamical isometry and a mean field theory of lstms and grus. *arXiv preprint arXiv:1901.08987*, 2019.

[73] Xavier Glorot and Yoshua Bengio. Understanding the difficulty of training deep feedforward neural networks. In *Proceedings of the thirteenth international conference on artificial intelligence and statistics*, pages 249–256, 2010.

[74] Xavier Glorot, Antoine Bordes, and Yoshua Bengio. Deep sparse rectifier neural networks. In *Proceedings of the fourteenth international conference on artificial intelligence and statistics*, pages 315–323, 2011.

[75] Ian Goodfellow, Yoshua Bengio, Aaron Courville, and Yoshua Bengio. *Deep learning*, volume 1. MIT press Cambridge, 2016.

[76] Ian J Goodfellow, Oriol Vinyals, and Andrew M Saxe. Qualitatively characterizing neural network optimization problems. *arXiv preprint arXiv:1412.6544*, 2014.

[77] Akhilesh Gotmare, Nitish Shirish Keskar, Caiming Xiong, and Richard Socher. A closer look at deep learning heuristics: Learning rate restarts, warmup and distillation. In *International Conference on Learning Representations*, 2019. URL `https://openreview.net/forum?id=r14EOsCqKX`.

[78] Priya Goyal, Piotr Dollár, Ross Girshick, Pieter Noordhuis, Lukasz Wesolowski, Aapo Kyrola, Andrew Tulloch, Yangqing Jia, and Kaiming He. Accurate, large minibatch sgd: Training imagenet in 1 hour. *arXiv preprint arXiv:1706.02677*, 2017.

[79] Vineet Gupta, Tomer Koren, and Yoram Singer. Shampoo: Preconditioned stochastic tensor optimization. *arXiv preprint arXiv:1802.09568*, 2018.

[80] Benjamin D Haeffele and René Vidal. Global optimality in neural network training. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 7331–7339, 2017.

[81] Song Han, Huizi Mao, and William J Dally. Deep compression: Compressing deep neural networks with pruning, trained quantization and huffman coding. *arXiv preprint arXiv:1510.00149*, 2015.

[82] Boris Hanin. Which neural net architectures give rise to exploding and vanishing gradients? In *Advances in Neural Information Processing Systems*, pages 580–589, 2018.

[83] Boris Hanin and David Rolnick. How to start training: The effect of initialization and architecture. In *Advances in Neural Information Processing Systems*, pages 569–579, 2018.

[84] Haowei He, Gao Huang, and Yang Yuan. Asymmetric valleys: Beyond sharp and flat local minima. *arXiv preprint arXiv:1902.00744*, 2019.

[85] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In *Proceedings of the IEEE international conference on computer vision*, pages 1026–1034, 2015.

[86] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 770–778, 2016.

[87] Geoffrey E Hinton and Ruslan R Salakhutdinov. Reducing the dimensionality of data with neural networks. *science*, 313(5786):504–507, 2006.

[88] Sepp Hochreiter and Jürgen Schmidhuber. Flat minima. *Neural Computation*, 9(1):1–42, 1997.

[89] Gao Huang, Zhuang Liu, Laurens Van Der Maaten, and Kilian Q Weinberger. Densely connected convolutional networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 4700–4708, 2017.

[90] Sergey Ioffe and Christian Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. *arXiv preprint arXiv:1502.03167*, 2015.

[91] Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in neural information processing systems*, pages 8571–8580, 2018.

[92] Prateek Jain, Sham M Kakade, Rahul Kidambi, Praneeth Netrapalli, and Aaron Sidford. Accelerating stochastic gradient descent. *arXiv preprint arXiv:1704.08227*, 2017.

[93] Daniel Jakubovitz, Raja Giryes, and Miguel RD Rodrigues. Generalization error in deep learning. In *Compressed Sensing and Its Applications*, pages 153–193. Springer, 2019.

[94] Majid Janzamin, Hanie Sedghi, and Anima Anandkumar. Beating the perils of non-convexity: Guaranteed training of neural networks using tensor methods. *arXiv preprint arXiv:1506.08473*, 2015.

[95] Ziwei Ji and Matus Telgarsky. Gradient descent aligns the layers of deep linear networks. *arXiv preprint arXiv:1810.02032*, 2018.

[96] Xianyan Jia, Shutao Song, Wei He, Yangzihao Wang, Haidong Rong, Feihu Zhou, Liqiang Xie, Zhenyu Guo, Yuanzhou Yang, Liwei Yu, et al. Highly scalable deep learning training system with mixed-precision: Training imagenet in four minutes. *arXiv preprint arXiv:1807.11205*, 2018.

[97] Rie Johnson and Tong Zhang. Accelerating stochastic gradient descent using predictive variance reduction. In *Advances in neural information processing systems*, pages 315–323, 2013.

[98] Sun Ju. List of works on "provable nonconvex methods/algorithms". *https://sunju.org/research/nonconvex/*.

[99] Kenji Kawaguchi. Deep learning without poor local minima. In *Advances in neural information processing systems*, pages 586–594, 2016.

[100] Kenji Kawaguchi and Leslie Pack Kaelbling. Elimination of all bad local minima in deep learning. *arXiv preprint arXiv:1901.00279*, 2019.

[101] Nitish Shirish Keskar and Richard Socher. Improving generalization performance by switching from adam to sgd. *arXiv preprint arXiv:1712.07628*, 2017.

[102] Nitish Shirish Keskar, Dheevatsa Mudigere, Jorge Nocedal, Mikhail Smelyanskiy, and Ping Tak Peter Tang. On large-batch training for deep learning: Generalization gap and sharp minima. *arXiv preprint arXiv:1609.04836*, 2016.

[103] Rahul Kidambi, Praneeth Netrapalli, Prateek Jain, and Sham Kakade. On the insufficiency of existing momentum schemes for stochastic optimization. In *2018 Information Theory and Applications Workshop (ITA)*, pages 1–9. IEEE, 2018.

[104] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

[105] Jonas Kohler, Hadi Daneshmand, Aurelien Lucchi, Thomas Hofmann, Ming Zhou, and Klaus Neymeyr. Exponential convergence rates for batch normalization: The power of length-direction decoupling in non-convex optimization. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 806–815, 2019.

[106] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. In *Advances in neural information processing systems*, pages 1097–1105, 2012.

[107] Rohith Kuditipudi, Xiang Wang, Holden Lee, Yi Zhang, Zhiyuan Li, Wei Hu, Sanjeev Arora, and Rong Ge. Explaining landscape connectivity of low-cost solutions for multilayer nets. *arXiv preprint arXiv:1906.06247*, 2019.

[108] Thomas Laurent and James Brecht. Deep linear networks with arbitrary loss: All local minima are global. In *International Conference on Machine Learning*, pages 2908–2913, 2018.

[109] Thomas Laurent and James von Brecht. The multilinear structure of relu networks. *arXiv preprint arXiv:1712.10132*, 2017.

[110] Yann LeCun, Leon Bottou, Genevieve B Orr, and Klaus-Robert Müller. Efficient backprop. In *Neural Networks: Tricks of the Trade*, pages 9–50. Springer, 1998.

[111] Yann A LeCun, Léon Bottou, Genevieve B Orr, and Klaus-Robert Müller. Efficient backprop. In *Neural networks: Tricks of the trade*, pages 9–48. Springer, 2012.

[112] Jaehoon Lee, Lechao Xiao, Samuel Schoenholz, Yasaman Bahri, Roman Novak, Jascha Sohl-Dickstein, and Jeffrey Pennington. Wide neural networks of any depth evolve as linear models under gradient descent. In *Advances in neural information processing systems*, pages 8570–8581, 2019.

[113] Namhoon Lee, Thalaiyasingam Ajanthan, and Philip Torr. SNIP: SINGLE-SHOT NETWORK PRUNING BASED ON CONNECTION SENSITIVITY. In *International Conference on Learning Representations*, 2019. URL `https://openreview.net/forum?id=B1VZqjAcYX`.

[114] Dennis Leventhal and Adrian S Lewis. Randomized methods for linear constraints: convergence rates and conditioning. *Mathematics of Operations Research*, 35(3):641–654, 2010.

[115] Dawei Li, Tian Ding, and Ruoyu Sun. Over-parameterized deep neural networks have no strict local minima for any continuous activations. *arXiv preprint arXiv:1812.11039*, 2018.

[116] Hao Li, Zheng Xu, Gavin Taylor, Christoph Studer, and Tom Goldstein. Visualizing the loss landscape of neural nets. In *Advances in Neural Information Processing Systems*, pages 6391–6401, 2018.

[117] Ping Li and Phan-Minh Nguyen. On random deep weight-tied autoencoders: Exact asymptotic analysis, phase transitions, and implications to training.

[118] Yuanzhi Li and Yingyu Liang. Learning overparameterized neural networks via stochastic gradient descent on structured data. In *Advances in Neural Information Processing Systems*, pages 8168–8177, 2018.

[119] Yuanzhi Li and Yang Yuan. Convergence analysis of two-layer neural networks with relu activation. In *Advances in Neural Information Processing Systems*, pages 597–607, 2017.

[120] Zhiyuan Li, Ruosong Wang, Dingli Yu, Simon S. Du, Wei Hu, Ruslan Salakhutdinov, and Sanjeev Arora. Enhanced convolutional neural tangent kernels, 2019.

[121] Shiyu Liang, Ruoyu Sun, Jason D Lee, and R Srikant. Adding one neuron can eliminate all bad local minima. In *Advances in Neural Information Processing Systems*, pages 4355–4365, 2018.

[122] Shiyu Liang, Ruoyu Sun, Yixuan Li, and Rayadurgam Srikant. Understanding the loss surface of neural networks for binary classification. *arXiv preprint arXiv:1803.00909*, 2018.

[123] Shiyu Liang, Ruoyu Sun, and R Srikant. Revisiting landscape analysis in deep neural networks: Eliminating decreasing paths to infinity. *arXiv preprint arXiv:1912.13472*, 2019.

[124] Hongzhou Lin, Julien Mairal, and Zaid Harchaoui. A universal catalyst for first-order optimization. In *Advances in Neural Information Processing Systems*, pages 3384–3392, 2015.

[125] Chaoyue Liu and Mikhail Belkin. Accelerating sgd with momentum for over-parameterized learning, 2018.

[126] Chaoyue Liu and Mikhail Belkin. Mass: an accelerated stochastic method for over-parametrized learning. *arXiv preprint arXiv:1810.13395*, 2018.

[127] Zhuang Liu, Mingjie Sun, Tinghui Zhou, Gao Huang, and Trevor Darrell. Rethinking the value of network pruning. *arXiv preprint arXiv:1810.05270*, 2018.

[128] Roi Livni, Shai Shalev-Shwartz, and Ohad Shamir. On the computational efficiency of training neural networks. In *Advances in Neural Information Processing Systems*, pages 855–863, 2014.

[129] Ilya Loshchilov and Frank Hutter. Sgdr: Stochastic gradient descent with warm restarts. *arXiv preprint arXiv:1608.03983*, 2016.

[130] Cheng Lu, Zhibin Deng, Jing Zhou, and Xiaoling Guo. A sensitive-eigenvector based global algorithm for quadratically constrained quadratic programming. *Journal of Global Optimization*, pages 1–18, 2019.

[131] Haihao Lu and Kenji Kawaguchi. Depth creates no bad local minima. *arXiv preprint arXiv:1702.08580*, 2017.

[132] Ping Luo, Ruimao Zhang, Jiamin Ren, Zhanglin Peng, and Jingyu Li. Switchable normalization for learning-to-normalize deep representation. *IEEE transactions on pattern analysis and machine intelligence*, 2019.

[133] Zhi-Quan Luo. On the convergence of the lms algorithm with adaptive learning rate for linear feed-forward networks. *Neural Computation*, 3(2):226–245, 1991.

[134] Chao Ma, Lei Wu, et al. Analysis of the gradient descent algorithm for a deep neural network model with skip-connections. *arXiv preprint arXiv:1904.05263*, 2019.

[135] James Martens. Deep learning via hessian-free optimization. In *ICML*, volume 27, pages 735–742, 2010.

[136] James Martens. New insights and perspectives on the natural gradient method. *arXiv preprint arXiv:1412.1193*, 2014.

[137] James Martens and Roger Grosse. Optimizing neural networks with kronecker-factored approximate curvature. In *International conference on machine learning*, pages 2408–2417, 2015.

[138] Song Mei and Andrea Montanari. The generalization error of random features regression: Precise asymptotics and double descent curve. *arXiv preprint arXiv:1908.05355*, 2019.

[139] Song Mei, Andrea Montanari, and Phan-Minh Nguyen. A mean field view of the landscape of two-layers neural networks. *arXiv preprint arXiv:1804.06561*, 2018.

[140] Hiroaki Mikami, Hisahiro Suganuma, Yoshiki Tanaka, Yuichi Kageyama, et al. Massively distributed sgd: Imagenet/resnet-50 training in a flash. *arXiv preprint arXiv:1811.05233*, 2018.

[141] Tomas Mikolov, Kai Chen, Greg Corrado, and Jeffrey Dean. Efficient estimation of word representations in vector space. *arXiv preprint arXiv:1301.3781*, 2013.

[142] Dmytro Mishkin and Jiri Matas. All you need is a good init. *arXiv preprint arXiv:1511.06422*, 2015.

[143] Takeru Miyato, Toshiki Kataoka, Masanori Koyama, and Yuichi Yoshida. Spectral normalization for generative adversarial networks. *arXiv preprint arXiv:1802.05957*, 2018.

[144] Marco Mondelli and Andrea Montanari. On the connection between learning two-layers neural networks and tensor decomposition. *arXiv preprint arXiv:1802.07301*, 2018.

[145] Ari S Morcos, Haonan Yu, Michela Paganini, and Yuandong Tian. One ticket to win them all: generalizing lottery ticket initializations across datasets and optimizers. *arXiv preprint arXiv:1906.02773*, 2019.

[146] Y. Nesterov. Efficiency of coordiate descent methods on huge-scale optimization problems. *SIAM Journal on Optimization*, 22(2):341–362, 2012.

[147] Behnam Neyshabur, Russ R Salakhutdinov, and Nati Srebro. Path-sgd: Path-normalized optimization in deep neural networks. In *Advances in Neural Information Processing Systems*, pages 2422–2430, 2015.

[148] Behnam Neyshabur, Srinadh Bhojanapalli, David McAllester, and Nati Srebro. Exploring generalization in deep learning. In *Advances in Neural Information Processing Systems*, pages 5947–5956, 2017.

[149] Phan-Minh Nguyen. Mean field limit of the learning dynamics of multilayer neural networks. *arXiv preprint arXiv:1902.02880*, 2019.

[150] Quynh Nguyen. On connected sublevel sets in deep learning. *arXiv preprint arXiv:1901.07417*, 2019.

[151] Quynh Nguyen, Mahesh Chandra Mukkamala, and Matthias Hein. On the loss landscape of a class of deep neural networks with no bad local valleys. *arXiv preprint arXiv:1809.10749*, 2018.

[152] Maher Nouiehed and Meisam Razaviyayn. Learning deep models: Critical points and local openness. *arXiv preprint arXiv:1803.02968*, 2018.

[153] Roman Novak, Lechao Xiao, Yasaman Bahri, Jaehoon Lee, Greg Yang, Daniel A. Abolafia, Jeffrey Pennington, and Jascha Sohl-dickstein. Bayesian deep convolutional networks with many channels are gaussian processes. In *International Conference on Learning Representations*, 2019. URL `https://openreview.net/forum?id=B1g30j0qF7`.

[154] Roman Novak, Lechao Xiao, Jiri Hron, Jaehoon Lee, Alexander A Alemi, Jascha Sohl-Dickstein, and Samuel S Schoenholz. Neural tangents: Fast and easy infinite neural networks in python. *arXiv preprint arXiv:1912.02803*, 2019.

[155] Brendan O?donoghue and Emmanuel Candes. Adaptive restart for accelerated gradient schemes. *Foundations of computational mathematics*, 15(3):715–732, 2015.

[156] Francesco Orabona and Tatiana Tommasi. Training deep networks without learning rates through coin betting. In *Advances in Neural Information Processing Systems*, pages 2160–2170, 2017.

[157] A Emin Orhan and Xaq Pitkow. Skip connections eliminate singularities. *arXiv preprint arXiv:1701.09175*, 2017.

[158] Kazuki Osawa, Yohei Tsuji, Yuichiro Ueno, Akira Naruse, Rio Yokota, and Satoshi Matsuoka. Second-order optimization method for large mini-batch: Training resnet-50 on imagenet in 35 epochs. *arXiv preprint arXiv:1811.12019*, 2018.

[159] Samet Oymak and Mahdi Soltanolkotabi. Overparameterized nonlinear learning: Gradient descent takes the shortest path? *arXiv preprint arXiv:1812.10004*, 2018.

[160] Samet Oymak and Mahdi Soltanolkotabi. Towards moderate overparameterization: global convergence guarantees for training shallow neural networks. *arXiv preprint arXiv:1902.04674*, 2019.

[161] Rina Panigrahy, Ali Rahimi, Sushant Sachdeva, and Qiuyi Zhang. Convergence results for neural networks via electrodynamics. *arXiv preprint arXiv:1702.00458*, 2017.

[162] Barak A Pearlmutter. Fast exact multiplication by the hessian. *Neural computation*, 6(1):147–160, 1994.

[163] Jeffrey Pennington, Richard Socher, and Christopher Manning. Glove: Global vectors for word representation. In *Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP)*, pages 1532–1543, 2014.

[164] Jeffrey Pennington, Samuel Schoenholz, and Surya Ganguli. Resurrecting the sigmoid in deep learning through dynamical isometry: theory and practice. In *Advances in neural information processing systems*, pages 4785–4795, 2017.

[165] Jeffrey Pennington, Samuel S Schoenholz, and Surya Ganguli. The emergence of spectral universality in deep networks. *arXiv preprint arXiv:1802.09979*, 2018.

[166] Tomaso Poggio and Qianli Liao. *Theory II: Landscape of the empirical risk in deep learning*. PhD thesis, Center for Brains, Minds and Machines (CBMM), arXiv, 2017.

[167] Ben Poole, Subhaneil Lahiri, Maithra Raghu, Jascha Sohl-Dickstein, and Surya Ganguli. Exponential expressivity in deep neural networks through transient chaos. In *Advances in neural information processing systems*, pages 3360–3368, 2016.

[168] Michael James David Powell. Restart procedures for the conjugate gradient method. *Mathematical programming*, 12(1):241–254, 1977.

[169] Sashank J Reddi, Satyen Kale, and Sanjiv Kumar. On the convergence of adam and beyond. 2018.

[170] Grant M Rotskoff and Eric Vanden-Eijnden. Neural networks as interacting particle systems: Asymptotic convexity of the loss landscape and universal scaling of the approximation error. *arXiv preprint arXiv:1805.00915*, 2018.

[171] Sebastian Ruder. An overview of gradient descent optimization algorithms. *arXiv preprint arXiv:1609.04747*, 2016.

[172] Itay Safran and Ohad Shamir. Spurious local minima are common in two-layer relu neural networks. *arXiv preprint arXiv:1712.08968*, 2017.

[173] Tim Salimans and Durk P Kingma. Weight normalization: A simple reparameterization to accelerate training of deep neural networks. In *Advances in Neural Information Processing Systems*, pages 901–909, 2016.

[174] Shibani Santurkar, Dimitris Tsipras, Andrew Ilyas, and Aleksander Madry. How does batch normalization help optimization? In *Advances in Neural Information Processing Systems*, pages 2483–2493, 2018.

[175] Andrew M Saxe, James L McClelland, and Surya Ganguli. Exact solutions to the nonlinear dynamics of learning in deep linear neural networks. *arXiv preprint arXiv:1312.6120*, 2013.

[176] Tom Schaul, Sixin Zhang, and Yann LeCun. No more pesky learning rates. In *International Conference on Machine Learning*, pages 343–351, 2013.

[177] Mark Schmidt and Nicolas Le Roux. Fast convergence of stochastic gradient descent under a strong growth condition. *arXiv preprint arXiv:1308.6370*, 2013.

[178] Nicol N Schraudolph. Fast curvature matrix-vector products for second-order gradient descent. *Neural computation*, 14(7):1723–1738, 2002.

[179] Shai Shalev-Shwartz, Ohad Shamir, and Shaked Shammah. Failures of gradient-based deep learning. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 3067–3075. JMLR. org, 2017.

[180] Ohad Shamir. Exponential convergence time of gradient descent for one-dimensional deep linear neural networks. *arXiv preprint arXiv:1809.08587*, 2018.

[181] Justin Sirignano and Konstantinos Spiliopoulos. Mean field analysis of neural networks. *arXiv preprint arXiv:1805.01053*, 2018.

[182] Justin Sirignano and Konstantinos Spiliopoulos. Mean field analysis of deep neural networks, 2019.

[183] Prabhu Teja Sivaprasad, Florian Mai, Thijs Vogels, Martin Jaggi, and Francois Fleuret. On the tunability of optimizers in deep learning, 2019.

[184] Leslie N Smith. Cyclical learning rates for training neural networks. In *2017 IEEE Winter Conference on Applications of Computer Vision (WACV)*, pages 464–472. IEEE, 2017.

[185] Leslie N Smith and Nicholay Topin. Super-convergence: Very fast training of neural networks using large learning rates. *arXiv preprint arXiv:1708.07120*, 2017.

[186] Samuel L. Smith, Pieter-Jan Kindermans, and Quoc V. Le. Don't decay the learning rate, increase the batch size. In *International Conference on Learning Representations*, 2018. URL `https://openreview.net/forum?id=B1Yy1BxCZ`.

[187] Mahdi Soltanolkotabi, Adel Javanmard, and Jason D Lee. Theoretical insights into the optimization landscape of over-parameterized shallow neural networks. *IEEE Transactions on Information Theory*, 65(2):742–769, 2019.

[188] Daniel Soudry and Elad Hoffer. Exponentially vanishing sub-optimal local minima in multilayer neural networks. *arXiv preprint arXiv:1702.05777*, 2017.

[189] Suvrit Sra, Sebastian Nowozin, and Stephen J Wright. *Optimization for machine learning*. Mit Press, 2012.

[190] Rupesh Kumar Srivastava, Klaus Greff, and Jürgen Schmidhuber. Highway networks. *arXiv preprint arXiv:1505.00387*, 2015.

[191] Lili Su and Pengkun Yang. On learning over-parameterized neural networks: A functional approximation prospective. In *Advances in Neural Information Processing Systems*.

[192] Grzegorz Swirszcz, Wojciech Marian Czarnecki, and Razvan Pascanu. Local minima in training of deep networks. 2016.

[193] Christian Szegedy, Wei Liu, Yangqing Jia, Pierre Sermanet, Scott Reed, Dragomir Anguelov, Dumitru Erhan, Vincent Vanhoucke, and Andrew Rabinovich. Going deeper with convolutions. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 1–9, 2015.

[194] Conghui Tan, Shiqian Ma, Yu-Hong Dai, and Yuqiu Qian. Barzilai-borwein step size for stochastic gradient descent. In *Advances in Neural Information Processing Systems*, pages 685–693, 2016.

[195] Mingxing Tan and Quoc V Le. Efficientnet: Rethinking model scaling for convolutional neural networks. *arXiv preprint arXiv:1905.11946*, 2019.

[196] Wojciech Tarnowski, Piotr Warchoł, Stanisław Jastrz?bski, Jacek Tabor, and Maciej Nowak. Dynamical isometry is achieved in residual networks in a universal way for any activation function. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 2221–2230, 2019.

[197] Yuandong Tian. An analytical formula of population gradient for two-layered relu network and its applications in convergence and critical point analysis. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 3404–3413. JMLR. org, 2017.

[198] Yuandong Tian, Tina Jiang, Qucheng Gong, and Ari Morcos. Luck matters: Understanding training dynamics of deep relu networks. *arXiv preprint arXiv:1905.13405*, 2019.

[199] Tijmen Tieleman and Geoffrey Hinton. Lecture 6.5-rmsprop: Divide the gradient by a running average of its recent magnitude. *COURSERA: Neural networks for machine learning*, 4(2):26–31, 2012.

[200] Dmitry Ulyanov, Andrea Vedaldi, and Victor Lempitsky. Instance normalization: The missing ingredient for fast stylization. *arXiv preprint arXiv:1607.08022*, 2016.

[201] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Advances in Neural Information Processing Systems*, pages 5998–6008, 2017.

[202] Sharan Vaswani, Francis Bach, and Mark Schmidt. Fast and faster convergence of sgd for over-parameterized models and an accelerated perceptron. *arXiv preprint arXiv:1810.07288*, 2018.

[203] Santosh Vempala and John Wilmes. Polynomial convergence of gradient descent for training one-hidden-layer neural networks. *arXiv preprint arXiv:1805.02677*, 2018.

[204] Luca Venturi, Afonso Bandeira, and Joan Bruna. Neural networks with finite intrinsic dimension have no spurious valleys. *arXiv preprint arXiv:1802.06384*, 15, 2018.

[205] Luca Venturi, Afonso Bandeira, and Joan Bruna. Spurious valleys in two-layer neural network optimization landscapes. *arXiv preprint arXiv:1802.06384*, 2018.

[206] Rene Vidal, Joan Bruna, Raja Giryes, and Stefano Soatto. Mathematics of deep learning. *arXiv preprint arXiv:1712.04741*, 2017.

[207] Gang Wang, Georgios B Giannakis, and Jie Chen. Learning relu networks on linearly separable data: Algorithm, optimality, and generalization. *arXiv preprint arXiv:1808.04685*, 2018.

[208] Rachel Ward, Xiaoxia Wu, and Leon Bottou. Adagrad stepsizes: Sharp convergence over nonconvex landscapes, from any initialization. *arXiv preprint arXiv:1806.01811*, 2018.

[209] Colin Wei, Jason D Lee, Qiang Liu, and Tengyu Ma. On the margin theory of feedforward neural networks. *arXiv preprint arXiv:1810.05369*, 2018.

[210] Francis Williams, Matthew Trager, Claudio Silva, Daniele Panozzo, Denis Zorin, and Joan Bruna. Gradient dynamics of shallow univariate relu networks, 2019.

[211] Ashia C Wilson, Rebecca Roelofs, Mitchell Stern, Nati Srebro, and Benjamin Recht. The marginal value of adaptive gradient methods in machine learning. In *Advances in Neural Information Processing Systems*, pages 4148–4158, 2017.

[212] Stephen Wright and Jorge Nocedal. Numerical optimization. *Springer Science*, 35(67-68):7, 1999.

[213] Lei Wu, Zhanxing Zhu, et al. Towards understanding generalization of deep learning: Perspective of loss landscapes. *arXiv preprint arXiv:1706.10239*, 2017.

[214] Yuxin Wu and Kaiming He. Group normalization. *ECCV*, 2018.

[215] Lechao Xiao, Yasaman Bahri, Jascha Sohl-Dickstein, Samuel S Schoenholz, and Jeffrey Pennington. Dynamical isometry and a mean field theory of cnns: How to train 10,000-layer vanilla convolutional neural networks. *arXiv preprint arXiv:1806.05393*, 2018.

[216] Saining Xie, Ross Girshick, Piotr Dollár, Zhuowen Tu, and Kaiming He. Aggregated residual transformations for deep neural networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 1492–1500, 2017.

[217] Yi Xu, Jing Rong, and Tianbao Yang. First-order stochastic algorithms for escaping from saddle points in almost linear time. In *Advances in Neural Information Processing Systems*, pages 5535–5545, 2018.

[218] Masafumi Yamazaki, Akihiko Kasagi, Akihiro Tabuchi, Takumi Honda, Masahiro Miwa, Naoto Fukumoto, Tsuguchika Tabaru, Atsushi Ike, and Kohta Nakashima. Yet another accelerated sgd: Resnet-50 training on imagenet in 74.7 seconds. *arXiv preprint arXiv:1903.12650*, 2019.

[219] Ge Yang and Samuel Schoenholz. Mean field residual networks: On the edge of chaos. In *Advances in neural information processing systems*, pages 7103–7114, 2017.

[220] Greg Yang. Scaling limits of wide neural networks with weight sharing: Gaussian process behavior, gradient independence, and neural tangent kernel derivation. *arXiv preprint arXiv:1902.04760*, 2019.

[221] Mingyang Yi, Qi Meng, Wei Chen, Zhi-ming Ma, and Tie-Yan Liu. Positively scale-invariant flatness of relu neural networks. *arXiv preprint arXiv:1903.02237*, 2019.

[222] Chris Ying, Sameer Kumar, Dehao Chen, Tao Wang, and Youlong Cheng. Image classification at supercomputer scale. *arXiv preprint arXiv:1811.06992*, 2018.

[223] Yang You, Zhao Zhang, Cho-Jui Hsieh, James Demmel, and Kurt Keutzer. Imagenet training in minutes. In *Proceedings of the 47th International Conference on Parallel Processing*, page 1. ACM, 2018.

[224] Jiahui Yu and Thomas Huang. Network slimming by slimmable networks: Towards one-shot architecture search for channel numbers. *arXiv preprint arXiv:1903.11728*, 2019.

[225] X. Yu and S. Pasupathy. Innovations-based MLSE for Rayleigh flat fading channels. *IEEE Transacations on Communications*, pages 1534–1544, 1995.

[226] Ya-xiang Yuan. Step-sizes for the gradient method. *AMS IP Studies in Advanced Mathematics*, 42(2): 785, 2008.

[227] Chulhee Yun, Suvrit Sra, and Ali Jadbabaie. Global optimality conditions for deep neural networks. *arXiv preprint arXiv:1707.02444*, 2017.

[228] Chulhee Yun, Suvrit Sra, and Ali Jadbabaie. Small nonlinearities in activation functions create bad local minima in neural networks. *arXiv preprint arXiv:1802.03487*, 2018.

[229] Matthew D Zeiler. Adadelta: an adaptive learning rate method. *arXiv preprint arXiv:1212.5701*, 2012.

[230] Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning requires rethinking generalization. *arXiv preprint arXiv:1611.03530*, 2016.

[231] Hongyi Zhang, Yann N Dauphin, and Tengyu Ma. Fixup initialization: Residual learning without normalization. *arXiv preprint arXiv:1901.09321*, 2019.

[232] Huishuai Zhang, Da Yu, Wei Chen, and Tie-Yan Liu. Training over-parameterized deep resnet is almost as easy as training a two-layer network. *arXiv preprint arXiv:1903.07120*, 2019.

[233] Li Zhang. Depth creates no more spurious local minima. *arXiv preprint arXiv:1901.09827*, 2019.

[234] Xiao Zhang, Yaodong Yu, Lingxiao Wang, and Quanquan Gu. Learning one-hidden-layer relu networks via gradient descent. *arXiv preprint arXiv:1806.07808*, 2018.

[235] Kai Zhong, Zhao Song, Prateek Jain, Peter L Bartlett, and Inderjit S Dhillon. Recovery guarantees for one-hidden-layer neural networks. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 4140–4149. JMLR. org, 2017.

[236] Dongruo Zhou, Yiqi Tang, Ziyan Yang, Yuan Cao, and Quanquan Gu. On the convergence of adaptive gradient methods for nonconvex optimization. *arXiv preprint arXiv:1808.05671*, 2018.

[237] Hattie Zhou, Janice Lan, Rosanne Liu, and Jason Yosinski. Deconstructing lottery tickets: Zeros, signs, and the supermask. *arXiv preprint arXiv:1905.01067*, 2019.

[238] Yi Zhou and Yingbin Liang. Critical points of neural networks: Analytical forms and landscape properties. *arXiv preprint arXiv:1710.11205*, 2017.

[239] Yi Zhou and Yingbin Liang. Critical points of linear neural networks: Analytical forms and landscape properties. 2018.

[240] Barret Zoph and Quoc V Le. Neural architecture search with reinforcement learning. *arXiv preprint arXiv:1611.01578*, 2016.

[241] Difan Zou, Yuan Cao, Dongruo Zhou, and Quanquan Gu. Stochastic gradient descent optimizes over-parameterized deep relu networks. *arXiv preprint arXiv:1811.08888*, 2018.

[242] Fangyu Zou and Li Shen. On the convergence of adagrad with momentum for training deep neural networks. *arXiv preprint arXiv:1808.03408*, 2018.

[243] Fangyu Zou, Li Shen, Zequn Jie, Weizhong Zhang, and Wei Liu. A sufficient condition for convergences of adam and rmsprop. *arXiv preprint arXiv:1811.09358*, 2018.