Effects of Depth, Width, and Initialization: A Convergence Analysis of Layer-wise Training for Deep Linear Neural Networks

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Abstract

Deep neural networks have been used in various machine learning applications and achieved tremendous empirical successes. However, training deep neural networks is a challenging task. Many alternatives have been proposed in place of end-to-end back-propagation. Layer-wise training is one of them, which trains a single layer at a time, rather than trains the whole layers simultaneously. In this paper, we study a layer-wise training using a block coordinate gradient descent (BCGD) for deep linear networks. We establish a general convergence analysis of BCGD and found the optimal learning rate, which results in the fastest decrease in the loss. More importantly, the optimal learning rate can directly be applied in practice, as it does not require any prior knowledge. Thus, tuning the learning rate is not needed at all. Also, we identify the effects of depth, width, and initialization in the training process. We show that when the orthogonal-like initialization is employed, the width of intermediate layers plays no role in gradient-based training, as long as the width is greater than or equal to both the input and output dimensions. We show that under some conditions, the deeper the network is, the faster the convergence is guaranteed. This implies that in an extreme case, the global optimum is achieved after updating each weight matrix only once. Besides, we found that the use of deep networks could drastically accelerate convergence when it is compared to those of a depth 1 network, even when the computational cost is considered. Numerical examples are provided to justify our theoretical findings and demonstrate the performance of layer-wise training by BCGD.

Keywords: Deep Linear Neural Networks, Layer-wise Training, Block Coordinate Gradient Descent, Convergence Analysis, Optimal Learning Rate

1. Introduction

Deep learning has drawn a lot of attention from both academia and industry due to its tremendous empirical success in various applications (Krizhevsky et al., 2012; Hinton et al., 2012; Silver et al., 2016; Wu et al., 2016). One of the key components in the success of deep learning is the intriguing ability of gradient-based optimization methods. Despite of the non-convex and non-smooth nature of the loss function, it somehow finds a local (or global) minimum, which performs well in practice. Mathematical analysis of this phenomenon has been undertaken. There are several theoretical works, which show that under the assumption of over-parameterization, more precisely, very wide networks, the (stochastic) gradient
descent algorithm finds a global minimum (Allen-Zhu et al., 2018; Du et al., 2018a, b; Zou et al., 2018; Oymak and Soltanolkotabi, 2019). These theoretical progresses have its own importance, however, it does not directly help practitioners to have better training results. This is mainly because there are still many parameters to be determined a priori: learning rate, the depth of network, the width of intermediate layers, optimization algorithms with its own internal parameters, to name just a few. The learning rates from existing theoretical works are not applicable in practice. For example, when a fully-connected ReLU network of depth 10 is trained over 1,000 training data, theoretically guaranteed learning rate is either \( \eta \approx \frac{1}{1000^{2/10}} \approx 10^{-5} \) (Du et al., 2018a) or \( \eta \approx \frac{1}{1000^{4/10}} \approx 10^{-14} \) (Allen-Zhu et al., 2018). Thus, practitioners typically choose these aforementioned parameters by either a grid search or trial and error.

Despite its expressive power, training deep neural networks is not an easy task. It has been widely known that the deeper the network is, the harder it is to be trained (Srivastava et al., 2015). Empirical success of deep learning heavily relies on numerous engineering tricks used in the training process. These includes but not limited to dropout (Srivastava et al., 2014), dropconnect (Wan et al., 2013), batch-normalization (Ioffe and Szegedy, 2015), weight-normalization (Salimans and Kingma, 2016), pre-training (Dahl et al., 2011), and data augmentation (Ciresan et al., 2012). Although these techniques are shown to be effective in many machine learning applications, it lacks rigorous justifications and hinders a thorough mathematical understanding of the training process of deep learning. The layer-wise training is an alternative to the standard end-to-end back-propagation, especially for training deep neural networks. The underlying principle is to train only a few layers (or a single layer) at a time, rather than train the whole layers simultaneously. This approach is not new and has been proposed in several different contexts. One stream of layer-wise training is adaptive training. At each stage, only a few layers (or a single) are trained. Once training is done, new layers are added. By fixing all the previously trained layers for the rest of the training, only newly added layers are trained. This procedure is repeated. The works of this direction include (Fahlman and Lebiere, 1990; Lengellé and Denoeux, 1996; Kulkarni and Karande, 2017; Belilovsky et al., 2018; Marquez et al., 2018; Malach and Shalev-Shwartz, 2018; Mosca and Magoulas, 2017; Huang et al., 2017). Another stream of layer-wise training is the block coordinate descent (BCD) method (Zhang and Brand, 2017; Zeng et al., 2018; Carreira-Perpinan and Wang, 2014; Askari et al., 2018; Gu et al., 2018; Lau et al., 2018; Taylor et al., 2016). The BCD is a Gauss-Seidel type of gradient-free methods, which trains each layer at a time by freezing all other layers, in a sequential order. Thus, all layers are updated once in every sweep of training. This paper concerns with the layer-wise training in this line of approach. In (Hinton and Salakhutdinov, 2006; Bengio et al., 2007), layer-wise training is employed as a pretraining strategy.

Deep linear network (DLN) is a neural network that uses linear activation functions. Although DLN is not a popular choice in practice, it is an active research subject as it is a class of decent simplified models for understanding the deep neural network with non-linear activation functions (Saxe et al., 2013; Hardt and Ma, 2016; Arora et al., 2018a, b; Bartlett et al., 2019). DLN has a trivial representation power (product of weight matrices), however, its training process is not trivial at all. It has been studied the loss surface of DLNs (Lu and Kawaguchi, 2017; Kawaguchi, 2016; Laurent and Brecht, 2018) and it is shown that although the loss surface is not convex, there are no spurious local minima. That is, all of
the local minima of DLNs are global minima. The work of (Arora et al., 2018a) studied a convergence analysis of gradient descent for DLNs. It shows that under the assumptions of whitened data, balanced initialization, deficiency margin, and sufficiently small learning rates, the vanilla gradient descent finds a global optimum. However, the learning rate from the analysis is not applicable in practice as it requires prior knowledge of the global minimizer. The theoretically guaranteed learning rate of (Arora et al., 2018a) should meet
\[ \eta \leq \frac{c(4L-2)/L}{6144L^3\|W^*\|_F^6(6L-4)/L}, \]
where \( W^* \) is the global minimizer, \( c \) is a constant related to the initial error, and \( L \) is the depth. Examples of (Arora et al., 2018a) use the learning rate from a grid search.

In this paper, we study a layer-wise training for DLNs using a block coordinate gradient descent (BCGD) (Tseng and Yun, 2009b, a). Similar to BCD, the BCGD trains each layer at a time in a sequential order by freezing all other layers at their last updated values. However, a key difference is the use of gradient descent in every update. Thus, the BCGD is a gradient-based optimization method. We establish a general convergence analysis and found the optimal learning rate, which leads to the fastest decrease in the loss. More importantly, the optimal learning rate can directly be applied in practice. We also identify the effects of depth, width, and initialization in the training process. When the orthogonal-like initialization is employed, as long as the width of intermediate layers is greater than or equal to both the input and output dimensions, the width plays no role in any gradient-based training. Also, we rigorously show that when (i) the orthogonal-like initialization is used, (ii) the initial loss is sufficiently small, the deeper the network is, the faster the convergence is guaranteed. Here, the speed of convergence is based on the number of sweeps, not the amount of computation. We remark that this criterion is commonly adopted in the literature (Saxe et al., 2013; Arora et al., 2018b). In an extreme case where the depth is sufficiently large, the convergence to the global optimum is guaranteed by updating each weight matrix only once. Similar behavior was empirically reported in (Arora et al., 2018b) as implicit acceleration. We emphasize that our analysis reveals the optimal learning rate and the effects of depth, width, and initialization in the training process. Therefore, neither trial and error nor a grid search for tuning parameters are required (especially, learning rate). Furthermore, we found that a well-chosen depth could result in a significant acceleration in convergence when it is compared to those of a single layer, even when the computational cost is considered. This clearly demonstrates the benefit of using deep networks (over-parameterization via depth). We also establish a convergence analysis of the block coordinate stochastic gradient descent (BCSGD). Our analysis indicates that the BCSGD cannot reach the global optimum, however, the converged loss will be staying close to the global optimum. This can be understood as an implicit regularization, which avoids over-fitting, due to the stochasticity introduced by the random selection of mini-batch. Numerical examples are provided to justify our theoretical findings and demonstrate the performance of layer-wise training by BCGD.

The rest of paper is organized as follows. In Section 2, we present the mathematical setup and introduce the block coordinate (stochastic) gradient descent. We then present a general convergence analysis and the optimal learning rate in Section 3. In Section 4, several numerical examples using both synthetic and real data sets are presented to demonstrate the effectiveness of the layer-wise training by BCGD and justify our theoretical findings.
2. Setup and Preliminary

Let $\mathcal{N}^L : \mathbb{R}^{d_{in}} \to \mathbb{R}^{d_{out}}$ be a feed-forward linear neural network with $L$ layers and having $n_\ell$ neurons in the $\ell$-th layer. We denote the weight matrix in the $\ell$-th layer by $W_\ell \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$. Here $n_0 = d_{in}$ and $n_L = d_{out}$. Let $\theta = \{W_\ell\}_{\ell=1}^L$ be the set of all weight matrices. Then the $L$-layer linear neural network can be written as

$$\mathcal{N}^L(x; \theta) = W_L W_{L-1} \cdots W_1 x.$$ 

Given a set of training data $\mathcal{T} = \{(x^i, y^i)\}_{i=1}^m$, the goal is to learn the parameters $\{W_\ell\}_{\ell=1}^L$ which minimize the loss function $L(\theta)$ defined by

$$L(\theta) = \sum_{i=1}^m L_i(\theta), \quad L_i(\theta) = \sum_{j=1}^{d_{out}} \ell(\mathcal{N}_j^L(x^i; \theta); y^i_j).$$

(1)

Here $\ell(a; b)$ is a metric which measures the discrepancy between the prediction and the output data. For example, the choice of $\ell(a; b) = (a - b)^p/p$ results in the standard $L_p$-loss function.

For a matrix $A \in \mathbb{R}^{m \times n}$, the spectral norm, the condition number and the scaled condition number are defined to be

$$\|A\| = \max_{\|x\|_2=1} \|Ax\|_2, \quad \kappa_r(A) = \frac{\sigma_{\max}(A)}{\sigma_r(A)}, \quad \tilde{\kappa}(A) = \frac{\|A\|_F}{\|A^{-1}\|_F},$$

respectively. Here $\| \cdot \|_2$ is the Euclidean norm, $\| \cdot \|_F$ is the Frobenius norm, $\sigma_{\max}()$ is the largest singular value, and $\sigma_r(\cdot)$ is the $r$-th largest singular value. Also, we denote the min$\{m, n\}$-th largest singular value by $\sigma_{\min}(\cdot)$. When $r = \min\{m, n\}$, we simply write the condition number as $\kappa(\cdot)$. The matrix $L_{p,q}$ norm is defined by

$$\|A\|_{p,q} = \left( \sum_{j=1}^n \left( \sum_{i=1}^m |a_{ij}|^p \right)^{q/p} \right)^{1/q}, \quad p, q \geq 1,$$

and the max norm is $\|A\|_{\max} = \max_{i,j} |a_{ij}|$.

2.1 Global minimum of $L_2$ loss

Since this paper mainly concerns with the standard $L_2$-loss, here we discuss its global minimum, which depends on the network architecture being used. Let $X = [x^1, \cdots, x^m] \in \mathbb{R}^{n_0 \times m}$ be the input data matrix and $Y = [y^1, \cdots, y^m] \in \mathbb{R}^{n_L \times m}$ be the output data matrix. Then, the problem of minimizing the $L_2$-loss function is

$$\min_{W_j \in \mathbb{R}^{n_j \times n_{j-1}}, 1 \leq j \leq L} \|W_{L:1} X - Y\|^2_F, \quad \text{where} \quad W_{L:1} := W_L \cdots W_1.$$ 

(2)

This problem is closely related to

$$\min_{W \in \mathbb{R}^{n_L \times n_0}} \|WX - Y\|^2_F, \quad \text{subject to} \quad \text{rank}(W) \leq \min\{n_0, \cdots, n_L\}.$$ 

(3)
Since the rank of $W_{L:1}$ is at most $n^*: = \min\{n_0, \cdots, n_L\}$, the minimized losses from (2) and (3) should be the same. Thus, if $\{W_{\ell:L}^*\}_{\ell=1}^L$ is a solution of (2), $W_{L:1}^*$ should be a global minimizer of (3). Therefore, a global minimizer of (2) and its corresponding minimized loss can be understood through (3). Thus, in what follows, we briefly discuss the solutions of (3).

Without the rank constraint, the solution of (3) is

$$W_{\text{gen}}^* = YX^\dagger + M(XX^\dagger - I_n), \quad \forall M \in \mathbb{R}^{nL \times n_0},$$

where $I_n$ is the identity matrix of size $n \times n$ and $X^\dagger$ is the Moore-Pensore pseudo-inverse of $X$. Assuming $X$ is a full row rank matrix, we have $W^* = YX^\dagger$, which allows an explicit formula $W^*_{LSQ} = YX^T(XX^T)^{-1}$. If $X$ is not a full row rank matrix, (3) allows infinitely many solutions. In this case, the least norm solution is often sought and it is $W^* = YX^\dagger$. Also, for any $W$, the following holds:

$$\mathcal{L}(W) = \|WX - Y\|^2_F = \|WX - W^*X\|^2_F + \mathcal{L}(W^*).$$

Thus, the minimizing $L_2$-loss is equivalent to minimizing $\|WX - W^*X\|^2_F$. Furthermore, for whitened data, the least norm solution is simply $W^* = YX^T$.

With the rank constraint, we consider two cases. If $\text{rank}(YX^\dagger) \leq n^*$, the rank constraint plays no role in the minimization. Thus, the global minimizer is (4). Let us consider the case of $\text{rank}(YX^\dagger) > n^*$. Let $r_x = \text{rank}(X)$, and $X = U_x\Sigma_xV_x^T$ be a compact singular value decomposition (SVD) of $X$ where only $r_x$ left-singular vectors and $r_x$ right-singular vectors corresponding to the non-zero singular values are calculated. Then, $X^\dagger = V_x\Sigma_x^{-1}U_x^T$ and it can be checked that $\text{rank}(YV_x^\dagger) = r^* = \text{rank}(YX^\dagger)$. Let $YV_x = \hat{U}_y\hat{\Sigma}_y\hat{V}_y^T$ be a compact SVD of $YV_x$. It then can be shown that the problem (3) is equivalent to

$$\min_{\mathcal{Z}} \|\mathcal{Z} - YV_x\|_F, \quad \text{subject to } \text{rank}(\mathcal{Z}) \leq n^*.$$  

To be more precise, if $Z^*$ is a solution (the best $n^*$-rank approximation to $YV_x$) to the above, $W^* = Z^*\Sigma_x^{-1}U_x^T$ is a solution of (3), which can be explicitly written as

$$W^* = \hat{U}_y\Sigma^x\hat{V}_y^T\Sigma_x^{-1}U_x^T, \quad \Sigma^x = \begin{bmatrix} D_s & 0 \\ 0 & 0 \end{bmatrix},$$

where $s = \min\{n^*, r^*\}$ and $D_s$ is the principal submatrix consisting of the first $s$ rows and columns of $\Sigma_y$. We remark that in general, (5) and the best $n^*$-rank approximation to $YX^\dagger$ are not the same.

### 2.2 Gradient-based Optimizations

Gradient-based optimization methods require the gradient of the loss function at every iteration. For reader’s convenience, here we present the calculation of the gradient. First, let us define the Jacobian matrix $J \in \mathbb{R}^{m \times d_{\text{out}}}$,

$$J^{(k)} = [J_{ij}^{(k)}], \quad J_{ij}^{(k)} = \ell'(N_j^{L}(x^i; \theta^{(k)}); y_{ij}^i), \quad 1 \leq i \leq m, 1 \leq j \leq d_{\text{out}}.$$  

Note that if $\ell(a, b) = (a - b)^2 / 2$, $J^{(k)} = (W_{L:1}^{(k)}X - Y)^T$. 

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Lemma 1 Let $\theta = \{W_\ell\}_{\ell=1}^L$ and $N^L(x; \theta) = W_L W_{L-1} \cdots W_1 x$, where $W_\ell \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$ for $1 \leq \ell \leq L$. Then
$$\frac{\partial L(\theta)}{\partial W_\ell} = (W_L \cdots W_{\ell+1})^T J^T (W_{\ell-1} \cdots W_1 X)^T.$$ 

Proof. Let us consider the case of $L = 2$. Let $\theta = \{W_2, W_1\}$, i.e., $N^2(x) = W_2 W_1 x$, where $W_1 \in \mathbb{R}^{n \times d_{in}}$, and $W_2 \in \mathbb{R}^{d_{out} \times n}$. For a matrix $M$, let us denote the $j$-th row of $M$ by $M_{(j,:)}$ and the $i$-th column of $M$ by $M_{(:,i)}$. Since $L = 2$, the loss function is $L(\theta) = \sum_{j=1}^{d_{out}} \sum_{i=1}^m \ell((W_2)_{(j,:)} W_1 x^i; y^i_j)$. The direct calculation shows that $\frac{\partial L(\theta)}{\partial (W_1)_{(i,:)}} = X J (W_2)_{(:,i)}$, which gives
$$\frac{\partial L(\theta)}{\partial (W_1)^T} = X J W_2, \quad \frac{\partial L(\theta)}{\partial (W_2)^T} = W_1 X J.$$ 

For general $L$, it readily follows from the case of $L = 2$ by letting $X \rightarrow W_{\ell-1} \cdots W_1 X$, $W_1 \rightarrow W_\ell$, and $W_2 \rightarrow W_L \cdots W_{\ell+1}$. 

We present four different gradient-based optimization methods; the standard gradient descent (GD), the block coordinate gradient descent (BCGD), the stochastic gradient descent (SGD), and the block coordinate stochastic gradient descent (BCSGD). All methods commence with an initialization $\theta^{(0)} = \{W_\ell^{(0)}\}_{\ell=1}^L$.

Let $k = (k_1, \ldots, k_L)$ be a multi-index, where each $k_\ell$ indicates the number of updates of the $\ell$-th layer weight matrix $W_\ell$. After the $k$-th iteration, we obtain a multi-index $k^{(k)} = (k_1^{(k)}, \ldots, k_L^{(k)})$ and its corresponding parameters are $\theta^{(k)} = \{W^{(k)}_\ell\}_{\ell=1}^L$. Given $k^{(k)} = (k_1^{(k)}, \ldots, k_L^{(k)})$, let
$$W_{i,j}^{(k)} := W_{i,j}^{(k_1^{(k)})} W_{i-1,j}^{(k_2^{(k)})} \cdots W_{j-1,j}^{(k_L^{(k)})}, \quad 1 \leq j < i \leq L.$$ 

If $k_\ell^{(k)} = k$ for all $j$, we write $W_{i,j}^{(k)} := W_{i,j}^{(k)} W_{i-1,j}^{(k)} \cdots W_{j-1,j}^{(k)}$ for $1 \leq j < i \leq L$. For notational completeness, we set $W_{i,j} = I$ whenever $i < j$. Also, we simply write $W_{L,1}^{(k)}$ as $W^{(k)}$.

- **Gradient Descent (GD):** The weight matrices are iteratively updated according to
$$W^{(k+1)}_\ell = W^{(k)}_\ell - \eta_k^{(k)} \left( \frac{\partial L(\theta)}{\partial W_\ell} \right)_{\theta = \theta^{(k)}} , \quad 1 \leq \ell \leq L$$
where $k = (k, \ldots, k)$. We remark that a single iteration of GD updates all weight matrices once.

- **Block Coordinate Gradient Descent (BCGD):** Let $i(\ell) = \ell$ if the ascending (bottom to top) ordering is employed and $i(\ell) = L - \ell + 1$ if the descending (top to bottom) ordering is employed. Let
$$k_{(k,0)} = k = (k, \ldots, k), \quad k_{(k,L)} = k_{k+1} = (k+1, \ldots, k+1),$$

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and \( e_j = (0, \cdots, 0, 1, 0, \cdots, 0) \). At the \((Lk + \ell)\)-th iteration, the \(i(\ell)\)-th layer weight matrix is updated according to

\[
W_{i(\ell)}^{(k+1)} = W_{i(\ell)}^{(k)} - \eta_{i(\ell)}^{k} \frac{\partial \mathcal{L}(\theta)}{\partial W_{i(\ell)}} \bigg|_{\theta=\theta^{k,\ell,\ell-1}},
\]

where \( k_{(k,\ell)} = k_{(k,\ell,\ell-1)} + e_{i(\ell)} \). Here

\[
\theta^{k,\ell,\ell-1} = \begin{cases} W_L^{(k)}, \cdots, W_{\ell}^{(k)}, W_{\ell-1}^{(k+1)}, \cdots, W_1^{(k+1)} & \text{if the ascending ordering is employed, and} \\ W_L^{(k+1)}, \cdots, W_{\ell-1}^{(k+1)}, W_{\ell}^{(k)}, \cdots, W_1^{(k)} & \text{if the descending ordering is employed.} \end{cases}
\]

if the ascending ordering is employed, and

if the descending ordering is employed. We refer the BCGD with the bottom to top (top to bottom) ordering as the ascending (descending) BCGD. Given a linear neural network of depth \( L \), a single sweep of the ascending (descending) BCGD consists of \( L \)-iterations starting from the first layer (the last layer) to the last layer (the first layer). That is, after a single sweep, all weight matrices are updated only once, in the order of from \( W_1 \) to \( W_L \) (\( W_L \) to \( W_1 \)). When \( L = 1 \), the BCGD is identical to GD.

We also remark that in order to update every weight matrix once, GD requires a single iteration and the BCGD requires a single sweep (\( L \)-iterations).

- **Stochastic Gradient Descent (SGD):** At the \((k+1)\)-th iteration, an index \( i_k \) is randomly chosen from \( \{1, \cdots, m\} \) and the weight matrices are updated according to

\[
W_{i(\ell)}^{(k+1)} = W_{i(\ell)}^{(k)} - \eta_{i(\ell)}^{k} \frac{\partial \mathcal{L}_{i(\ell)}(\theta)}{\partial W_{i(\ell)}} \bigg|_{\theta=\theta^{k}} , \quad 1 \leq \ell \leq L,
\]

where \( k = (k, \cdots, k) \).

- **Block Coordinate Stochastic Gradient Descent (BCSGD):** At the \((Lk + \ell)\)-th iteration, an index \( i_{k(k+1)} \) is randomly chosen from \( \{1, \cdots, m\} \) and the \(i(\ell)\)-th layer weight matrix is updated according to

\[
W_{i(\ell)}^{(k+1)} = W_{i(\ell)}^{(k)} - \eta_{i(\ell)}^{k,\ell,\ell-1} \frac{\partial \mathcal{L}_{i_{k(k+1)}}(\theta)}{\partial W_{i(\ell)}} \bigg|_{\theta=\theta^{k}} , \quad (7)
\]

where \( k_{(k,\ell)} = k_{(k,\ell,\ell-1)} + e_{i(\ell)} \). Again, when \( L = 1 \), the BCSGD is identical to SGD.

### 2.3 Initialization

Any gradient-based optimization starts with an initialization \( \theta^{k_0} = \{W_{\ell}^{(0)}\}_{\ell=1}^{L} \), where \( k_0 = (0, \cdots, 0) \). Here we present three initialization schemes for training DLNs.

Let \( A \) be a matrix of size \( m \times n \) and \( B \) be of size \( k \times s \) where \( m \geq k, n \geq s \). We say \( A \) is equivalent to \( B \) up to zero-valued padding if

\[
A = \begin{bmatrix} B & 0 \\ 0 & 0 \end{bmatrix},
\]

and e_j = (0, \cdots, 0, 1, 0, \cdots, 0). At the \((Lk + \ell)\)-th iteration, the \(i(\ell)\)-th layer weight matrix is updated according to
and write $A \cong B$. Suppose $\min\{m, n\} > k = s$. We then write $A \cong B$ if $A \cong \tilde{B}$ where $\tilde{B}$

\[
\tilde{B} = \begin{bmatrix}
B & 0 \\
0 & I_{\min\{m, n\} - k}
\end{bmatrix}.
\]

Here $I_n$ is the identity matrix of size $n$. We consider the following weight initialization

schemes.

- **Orthogonal Initialization** (Saxe et al., 2013): $W^{(0)}_j \cong Q_{j, \min\{n_j, n_{j-1}\}}$ for all $1 \leq j \leq L$, where $Q_n$ is an orthogonal matrix of size $n$.

- **Orth-Identity Initialization**: $W^{(0)}_j \cong I_{\min\{n_j, n_{j-1}\}}$ for $1 \leq j \leq L$.

- **Balanced Initialization** (Arora et al., 2018a): Given a randomly drawn matrix $W^{(0)} \in \mathbb{R}^{n_L \times n_0}$, let us take a singular value decomposition $W^{(0)} = U \Sigma V^T$, where $U \in \mathbb{R}^{n_L \times \min\{n_0, n_L\}}$, $\Sigma \in \mathbb{R}^{\min\{n_0, n_L\} \times \min\{n_0, n_L\}}$ is diagonal, and $V \in \mathbb{R}^{n_0 \times \min\{n_0, n_L\}}$ have orthogonal columns. Set $W^{(0)}_L \cong U \Sigma^{1/L}$, $W^{(0)}_j \cong \Sigma^{1/L}$ for $1 < j < L$, $W^{(0)}_1 \cong \Sigma^{1/L} V^T$.

- **Random Initialization**: $(W^{(0)}_{ij})_{ik} \sim N(0, \sigma^2_j)$ for all $1 \leq j \leq L$. Often $\sigma^2_j$ is chosen to $1/n_{j-1}$ so that the expected value of the square norm of each row is 1.

The orth-identity initialization can be viewed as a hybrid initialization between the orthogonal and the identity initialization schemes. This paper primarily concerns with the orth-identity initialization.

### 3. Convergence Analysis

In this section, we present a convergence analysis of BCGD and establish the optimal learning rate. The optimality is defined to be the learning rate which results in the fastest decrease in the loss at the current parameters. The standard $L_2$-loss will be mainly discussed. However, we also present a convergence result for general differentiable convex loss functions whose gradient are Lipschitz continuous in a bounded domain, such as $L_p$-loss where $p$ is even.

We measure the approximation error in terms of the distance to the global optimum. For example, when the $L_2$-loss is employed, the error is $\mathcal{L}(W^{k}) - \mathcal{L}(W^*) = \|W^{k}X - W^*X\|_2^2$.

We first identify the effects of width in DLNs in gradient-based training under either the orth-identity or the balanced (Arora et al., 2018a) initialization (Section 2.3).

**Theorem 2** Suppose the weight matrices are initialized according to either the orth-identity or the balanced initialization, described in Section 2.3. Let $n_\ell$ be the width of the $\ell$-th layer. Then, the training process of any gradient-based optimization methods (including GD, SGD, BCGD, BCSGD) is independent of the choice of $n_\ell$’s as long as it satisfies

\[
\min_{1 \leq \ell \leq L} n_\ell \geq \max\{n_0, n_L\}.
\]
The proof can be found in Appendix A.

Theorem 2 implies that the width does not play any role in gradient-based training if the condition of (8) is met and the weight matrices are initialized in a certain manner. However, the same conclusion does not follow if the random initialization is employed. This indicates that the role of width highly depends on how the weight matrices are initialized. Also, with a proper initialization, over-parameterization by the width can be avoided.

3.1 Convergence of BCGD

We first focus on the standard $L_2$ loss function and present a general convergence analysis of BCGD. We do not make any assumptions other than range($YX^\dagger$) $\subset$ range($W_L^{(0)}$). For example, the input data matrix $X$ needs not be full rank. We follow the convention of $0 \times \infty = \frac{1}{\infty} = 0 \times \frac{1}{0} = 0$.

Theorem 3 Let $\ell(z;b) = (z - b)^2/2$. Suppose all columns of $W_L^{(0)}$ are initialized to be in a subspace $K$ in $\mathbb{R}^{nL}$ such that range($YX^\dagger$) $\subset$ $K$. Then, the $k$-th sweep (the $kL$-th iteration) of BCGD (6) with the learning rates of

$$\eta^{k(s,\ell-1)}_{\ell} = \frac{\eta}{\|W_{L:((i\ell)+1)}^{k(s,\ell-1)}\|^2\|W_{L:((i\ell)-1):1}^{k(s,\ell-1)}\|^2}, \quad 0 < \eta < 2,$$

where $i(\ell) = \ell$ if the ascending BCGD is employed and $i(\ell) = L - \ell + 1$ if the descending BCGD is employed, satisfies

$$\mathcal{L}(W^k) - \mathcal{L}(W^*) \leq \left(\mathcal{L}(W^0) - \mathcal{L}(W^*)\right) \prod_{s=0}^{k-1} \prod_{\ell=1}^{L} \left(\gamma^{k(s,\ell-1)}\right)^2,$$

where $W^* = YX^\dagger$, $r_x = \text{rank}(X)$, $r = \text{dim}(K)$, and

$$\gamma^{k(s,\ell-1)} = \max\left\{1 - \frac{\eta}{\kappa_{\ell}(W_L^{k(s,\ell-1)})^2\kappa_{\ell}(W_L^{k(s,\ell-1)}:1)^2\|W_{L:((i\ell)+1):1}^{k(s,\ell-1)}\|^2\}, \eta - 1\right\}.$$

Furthermore, the optimal learning rate is

$$\eta_{\text{opt}}^{k(s,\ell-1)} = \frac{\left\|\frac{\partial \mathcal{L}}{\partial W_L^{k(s,\ell-1)}}|_{\theta = \theta^{k(s,\ell-1)}}\right\|^2_F}{\left\|W_{L:((i\ell)+1):1}^{k(s,\ell-1)}\right\|^2_F},$$

and with the optimal learning rate of (11), we obtain

$$\mathcal{L}(W^k) = \mathcal{L}(W^0) - \sum_{s=0}^{k-1} \sum_{\ell=1}^{L} \left\|\frac{\partial \mathcal{L}}{\partial W_L^{k(s,\ell-1)}}|_{\theta = \theta^{k(s,\ell-1)}}\right\|^4_F.$$
Proof The proof can be found in Appendix B.

The assumption of all columns of $W_L^{(0)}$ being in range($YX^T$) $\subset K$ is automatically satisfied if $n_{L-1} \geq n_L$ and $W_L^{(0)}$ is a full rank matrix. Also, since range($W_L^{(0)}$) affects the rate of convergence through $\kappa_r(W_L^{(k,\ell-1)})$, a faster convergence is expected if range($W_L^{(0)}$) = range($YX^T$). If $n_L > n_{L-1} \geq n_0$, the choice of $W_L^{(0)} \simeq Q$ satisfies this, where $Q$ is orthogonal and range($Q$) = range($YX^T$). We remark that in many practical applications, the number of training data is typically larger than both the input and the output dimensions, i.e., $m > \max\{n_0, n_L\}$. Also, the input dimension is greater than the output dimension, i.e., $n_0 > n_L$. For example, the MNIST handwritten digit dataset contains 60,000 training data whose input and output dimensions are 784 and 10, respectively.

Theorem 3 indicates that as long as $\eta \geq \min\{r_x, r\}$, the approximation error is strictly decreasing after a single sweep of BCGD if either $\kappa_r^2(W_L^{(k,\ell)})$ or $\sigma_r(W_L^{(k,\ell)})$ is positive. Also, our analysis shows the ineffectiveness of training a network which has a layer whose width is less than $\max\{r_x, r\}$. This is because if $\eta < \max\{r_x, r\}$, either $\sigma_r(W_L^{(k,\ell)})$ or $\sigma_r(W_L^{(k,\ell)})$ is zero and thus, $\gamma^{(k,\ell)} = 1$. This indicates that in order for the faster convergence, one should employ a network whose architecture satisfying $n_\ell \geq \max\{r_x, r\}$ for all $1 \leq \ell < L$. Also, if $W_1^{(0)}$ is initialize in a way that all rows are in range($X$), one can expect to find the least norm solution.

In order for an iteration of BCGD to strictly decrease the approximation error, it is important to guarantee the condition of

$$\sigma_r^2(W_L^{(k,\ell)}), \sigma_r^2(W_L^{(k,\ell-1)}X) > 0. \quad (12)$$

In what follows, we show that if the initial approximation error is sufficiently close to the global optimum under the orth-identity initialization (Section 2.3), the convergence to the global optimum is guaranteed at a linear rate by the layer-wise training (BCGD).

**Theorem 4** Under the same conditions of Theorem 3, let $X$ be a full-row rank matrix and $\eta = \max\{n_0, n_L\}$ for all $1 \leq \ell < L$. Suppose the weight matrices are initialized from the orth-identity initialization (Section 2.3) and the initial loss $\|W^0 - W^*\|_F$ is less than or equal to $\bar{\sigma}_{\min}/c$, where $\bar{\sigma}_{\min} = \sigma_{\min}(W^*X)/\|X\|$, then

$$c = 1 + \kappa^2(X) \left(1 + \sqrt{1 + 4h(L)\bar{\sigma}_{\min}/\kappa^2(X)} \right) / 2h(L)\bar{\sigma}_{\min}, \quad h(L) = \frac{LR_L(1 - R_L)^{2L-2}}{(1 + R_L)^{3L-1}}, \quad (13)$$

and $R_L = \frac{2}{(5L-3) + \sqrt{(5L-3)^2 - 4L}}$. Then, with the learning rates of (9), the $k$-th sweep of BCGD satisfies

$$\mathcal{L}(W_k^k) - \mathcal{L}(W^*) \leq \left(\mathcal{L}(W_0^k) - \mathcal{L}(W^*)\right) (\gamma^2)^k,$$

where $\gamma = 1 - \frac{\eta}{5\kappa^2(X)}$ and $0 < \eta \leq 1$.

**Proof** By Lemma 5, the proof readily follows from Theorem 3.
Lemma 5. Under the same conditions of Theorem 4, we have

\[ \gamma^{k(k,\ell-1)} < 1 - \frac{\eta}{\kappa^2(X)} \left( \frac{1 - R_L}{1 + R_L} \right)^{2(L-1)} \leq \gamma = 1 - \frac{\eta}{5\kappa^2(X)}. \]

Proof. The proof can be found in Appendix C.

We remark that the rate of convergence for a single sweep is \( \gamma^2L \). When the speed of convergence is measured against the number of sweeps, this implies that the deeper the network is, the faster convergence is obtained. Thus, if the depth of a linear network is sufficiently large, the global optimum can be reached by the layer-wise training (BCGD) after updating each weight matrix only once.

Theorem 4 relies on the assumption that the initial approximation is sufficiently close to the global optimum \( \mathbf{W}^* \) in terms of \( X, \sigma_{\text{min}}(\mathbf{W}^*X) \) and the depth \( L \). As a special case of \( d_{out} = 1 \), a similar result can be obtained without this restriction.

Theorem 6. Under the same conditions of Theorem 3, let \( n_L = 1, n_\ell \geq n_0 \) for all \( 1 \leq \ell < L \) and \( X \) is a full-row rank matrix. Suppose the weight matrices are initialized from the orth-identity initialization (Section 2.3), and the global minimizer is not \( \mathbf{W}^* \neq \mathbf{W}^{k(0,\ell-1)}(\mathbf{I}_{n_0} - \|\mathbf{X}\|^2(XX^T)^{-1}/\eta) \) for all \( 1 \leq \ell \leq L \), and the depth \( L \) is chosen to satisfy

\[ L \geq \frac{\log \left( \frac{\sigma_{\text{min}}(\mathbf{W}^*X)}{c\|\mathbf{W}^{k_0}-\mathbf{W}^*\|_F} \right)}{\log(1 - \eta/\kappa^2(X))}, \]

where \( c \) is defined in (13) and \( 0 < \eta \leq 1 \). Then, the \( k \)-th sweep of descending BCGD with the learning rate of (9) satisfies

\[ \mathcal{L}(\mathbf{W}^{k_0}) - \mathcal{L}(\mathbf{W}^*) < \left( \mathcal{L}(\mathbf{W}^{k_0}) - \mathcal{L}(\mathbf{W}^*) \right) \left( 1 - \frac{\eta}{\kappa^2(X)} \right)^{2(L+k-1)} \left( \gamma^{2(L-1)} \right)^{k-1}, \]

where \( \gamma = 1 - \frac{\eta}{5\kappa^2(X)} \).

Proof. The proof can be found in Appendix D.

We now present a general convergence analysis of the layer-wise training (BCGD) for convex differentiable loss functions. For general loss functions, let \( \mathbf{W}^* \) be the solution to \( \min_{\mathbf{W}} \mathcal{L}(\mathbf{W}) \).

Theorem 7. Suppose \( \ell(z;b) \) is convex and twice differentiable (as a function of \( z \)), and that its second derivative satisfies \( |\ell''(z;b)| \leq C(z) \). If the learning rates satisfy

\[ 0 < \eta_\ell^{k(k,\ell-1)} \leq \frac{1}{\|\mathcal{C}(\Delta^{k(k,\ell-1)})\|_{\text{max}}\|\mathbf{W}^{k(k,\ell-1)}_{L:((\ell-1)+1)}\|^2\|\mathbf{W}^{k(k,\ell-1)}_{((\ell-1)+1):\mathbf{X}}\|^2}, \]

(15)
where $\mathcal{C}$ is applied element-wise and $\Delta^{k_{(k,\ell-1)}} = W^{k_{(k,\ell-1)}} X - Y$, the $(Lk + \ell)$-th iteration of BCGD satisfies

$$
\mathcal{L}(\theta^{k_{(k,\ell-1)}}) \leq \mathcal{L}(\theta^{k_{(k,\ell-1)}}) - \frac{\eta_{\ell}}{2} \|J^{k_{(k,\ell-1)}}\|_F^2,
$$

where $J^{k_{(k,\ell-1)}} = \frac{\partial \mathcal{L}(\theta)}{\partial W_{\ell}(\ell)} \bigg|_{\theta = \theta^{k_{(k,\ell-1)}}} = (W^{k_{(k,\ell-1)}} X J^{k_{(k,\ell-1)}} W^{k_{(k,\ell-1)}})$. Furthermore,

- The (near) optimal learning rate is

$$
\frac{k_{(k,\ell-1)}}{\eta_{\text{opt}}} = \frac{\|J^{k_{(k,\ell-1)}}\|_F^2}{\|\mathbb{C}(J^{k_{(k,\ell-1)}})\|_{\max}} \left\| W_{L,(\ell-1):L}^{k_{(k,\ell-1)}} J^{k_{(k,\ell-1)}} W^k_{(\ell-1):1} \right\|_F^2.
$$

- For each $\ell$, $\lim_{k \to \infty} \eta_{\ell} k_{(k,\ell-1)} \|J^{k_{(k,\ell-1)}}\|_F^2 = 0$.

- $\frac{1}{k\ell} \sum_{s=0}^{k-1} \sum_{\ell=1}^{L} \|J^{k_{(k,\ell-1)}}\|_F^2 = O(\frac{1}{k\ell})$.

- If $0 < \inf_{k} \eta_{\ell} k_{(k,\ell-1)} \leq \sup_{k} \eta_{\ell} k_{(k,\ell-1)} \leq 1$, we have

$$
\lim_{k \to \infty} \|\eta_{\ell} k_{(k,\ell-1)} \|J^{k_{(k,\ell-1)}}\|_F^2 = 0, \quad \lim_{k \to \infty} \|J^{k_{(k,\ell-1)}}\|_F^2 = 0.
$$

Therefore, $\{W_{\ell}^{k_{(k,\ell-1)}}\}_{\ell=1}^{k \to \infty} \to \{\hat{W}_{\ell}\}_{\ell=1}$ and $\{\hat{W}_{\ell}\}_{\ell=1}$ is a stationary point. If $\hat{W}_{L:1}$ is a local minimum, then it is the global minimum.

**Proof** The proof can be found in Appendix E.

Theorem 7 shows that as long as the learning rates satisfying (15) are bounded below away from 0 and above by 1 for all $k$ but finitely many, the BCGD finds a stationary point at the rate of $O(1/kL)$ where $k$ is the number of sweeps and $L$ is the depth of DLN. Also, since the loss $\ell$ is known a priori, the (near) optimal learning rate can directly be applied in practice. For example, when the $p$-norm is used for the loss, i.e., $\ell(z; b) = |z - b|^p / p$ where $1 < p < \infty$ and $p$ is even, the (near) optimal learning rate is

$$
\frac{k_{(k,\ell-1)}}{\eta_{\text{opt}}} = \frac{\|J^{k_{(k,\ell-1)}}\|_F^2}{(p-1)\|\Delta^{k_{(k,\ell-1)}}\|_{\max}^2 \left\| W_{L,(\ell-1):1}^{k_{(k,\ell-1)}} J^{k_{(k,\ell-1)}} W_{(\ell-1):1}^{k} \right\|_F^2}.
$$

Note that when $p = 2$, the above is identical to the optimal learning rate of (11).

### 3.2 Convergence of BCSGD

In this subsection, a convergence analysis of BCSGD (7) is presented with the standard $L_2$-loss, i.e., $\ell(a; b) = (a - b)^2 / 2$.

Given a discrete random variable $i \sim \pi$ on $[m]$, we denote the expectation with respect to $i$ conditioned on all other previous random variables by $\mathbb{E}_i$. 

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Theorem 8 Let \( \{W^{(0)}_\ell\}_{\ell=1}^L \) be the initial weight matrices. At the \((Lk+\ell)\)-th iteration, a data point \(x_{i_{Lk+\ell}}\) is randomly independently chosen where \(i_{Lk+\ell}\) is a random variable whose probability distribution \(\pi_{k(Lk,\ell)}\) is defined by

\[
\pi_{k(Lk,\ell)}(i) = \frac{\|W_{(i-1);1}^{k(Lk,\ell-1)} x_i^T W_{(i-1);1}^{k(Lk,\ell-1)} X\|^2}{\|W_{(i-1);1}^{k(Lk,\ell-1)} X\|^2}, \quad 1 \leq i \leq m. \tag{19}
\]

Then, the approximation by BCSGD (7) with the learning rates of

\[
\eta_{i_{Lk+\ell}} = \frac{s^2_{\min}(\hat{W}_{(i-1);1}^{k(Lk,\ell-1)} X)}{s^2_{\max}(\hat{W}_{((i+1);1}^{k(Lk,\ell-1)} X)} \frac{\eta}{\|W_{(i-1);1}^{k(Lk,\ell-1)} x_i^T W_{(i-1);1}^{k(Lk,\ell-1)} X\|^2}, \quad 0 < \eta < 2, \tag{20}
\]

satisfies

\[
E_{i_{Lk+\ell}}[\|\Delta (k,\ell)\|^2_F] \leq \frac{k_{(Lk,\ell-1)} \|\Delta k_{(Lk,\ell-1)}\|^2_F}{\bar{\kappa}^4(W^{k(Lk,\ell-1)}_{((i+1);1} X)} + \frac{\eta^2 \mathcal{L}(W^*)}{\bar{\kappa}^4(W^{k(Lk,\ell-1)}_{(i-1);1} X)},
\]

\[
E_{i_{Lk+\ell}}[\|\Delta (k,\ell)\|^2_F] \geq \frac{k_{(Lk,\ell-1)} \|\Delta k_{(Lk,\ell-1)}\|^2_F}{\bar{\kappa}^4(W^{k(Lk,\ell-1)}_{((i+1);1} X)} + \frac{\eta^2 \mathcal{L}(W^*)}{\bar{\kappa}^4(W^{k(Lk,\ell-1)}_{((i-1);1} X)},
\]

where \(W^* = Y X^\dagger, \Delta k_{(k,\ell)} = W_{L;1}^{k(Lk,\ell)} X - W^* X\),

\[
\gamma_{\text{upp}}^{k(k,\ell-1)} = \max(1 - \left(1 - \frac{\eta^2 (W^{k,k(k,\ell-1)})_{((i+1);1} X)}{\bar{\kappa}^4(W^{k(k,\ell-1)}_{((i-1);1} X)}\right)^2, \gamma_{\text{low}}^{k(k,\ell-1)} = 1 - \left(1 - \frac{\eta^2 (W^{k(k,\ell-1)}_{((i+1);1} X)}{\bar{\kappa}^4(W^{k(k,\ell-1)}_{((i-1);1} X)}\right)^2).
\]

Proof The proof can be found in Appendix F.

Under the assumption that \(\kappa^4(W^{k(k,\ell-1)}_{((i+1);1} X)\), \(\kappa^4(W^{k(k,\ell-1)}_{((i-1);1} X)\) uniformly bounded above by \(M_{\text{upp}}\) and \(\gamma_{\text{low}}^{k(k,\ell-1)}\) is uniformly bounded below away from zero by \(\gamma_{\text{low}} > 0\), one can conclude that

\[
E[\|\Delta k^2\|^2_F] \geq \gamma_{\text{low}} \|\Delta k\|^2_F + \frac{\eta^2 \mathcal{L}(W^*)(1 - \gamma_{\text{low}}) \|\Delta k\|^2_F}{M_{\text{upp}}(1 - \gamma_{\text{low}})} \to \frac{\eta^2 \mathcal{L}(W^*)}{M_{\text{upp}}(1 - \gamma_{\text{low}})} \quad \text{as} \quad k \to \infty.
\]

Similarly, under the assumption that \(\bar{\kappa}^4(W_{((i+1);1}^{k(k,\ell-1)} X)\) uniformly bounded below by \(M_{\text{low}}\), and \(\gamma_{\text{upp}}^{k(k,\ell-1)}\) is uniformly bounded above by \(\gamma_{\text{upp}} < 1\), we have

\[
E[\|\Delta k^2\|^2_F] \leq \gamma_{\text{upp}} \|\Delta k\|^2_F + \frac{\eta^2 \mathcal{L}(W^*)(1 - \gamma_{\text{upp}}) \|\Delta k\|^2_F}{M_{\text{low}}(1 - \gamma_{\text{upp}})} \to \frac{\eta^2 \mathcal{L}(W^*)}{M_{\text{low}}(1 - \gamma_{\text{upp}})} \quad \text{as} \quad k \to \infty.
\]

This indicates that unlike the BCGD, if a randomly chosen datum is used to update a weight matrix, an extra term, which is proportional to \(\mathcal{L}(W^*)\), is introduced in both upper
and lower bounds of the expected error. Therefore, the BCSGD would not achieve the
global optimum, unless $\mathcal{L}(W^*) = 0$. However, the expected loss by BCSGD will be within
the distance proportional to $\mathcal{L}(W^*)$ from $\mathcal{L}(W^*)$. In practice, $\mathcal{L}(W^*)$ will almost never be
zero. This indicates that the stochasticity introduced by the random selection of mini-batch
(of size 1) results in an implicit regularization effect, which avoids over-fitting. We defer
further characterization of BCSGD to future work.

4. Numerical Examples

We provide numerical examples to demonstrate the performance of layer-wise training by
BCGD and justify our theoretical findings. We employ three different initialization schemes,
described in Section 2.3. In all examples, the network architectures are met the condition
of $n_\ell \geq \max\{d_{in}, d_{out}\}$ unless otherwise stated. According to Theorem 2, when either the
orth-identity or the balanced initialization is employed, we simply set $n_\ell = \max\{n_0, n_L\}$
for all $1 \leq \ell < L$. The approximation error is measured by the normalized distance to
the global optimum, i.e., $\frac{1}{m} \mathcal{L}(W^{(k)}) - \frac{1}{m} \mathcal{L}(W^*)$. When the $L_2$-loss is employed, the error
after the $k$-th sweep is $\frac{1}{m} \left[ \|W^{(k)}X - Y\|_F^2 - \|W^*X - Y\|_F^2 \right]$. We note that the speed of
convergence can be measured by either the number of sweeps or the number of iterations.
Note also that updating each weight matrix once in a deep network will require more time
than doing so in a shallow network. When it comes to compare the speed of convergence in
deep neural networks, the number of times each weight matrix is updated is a commonly
employed criterion (Saxe et al., 2013; Arora et al., 2018b).

In what follows, we employ the layer-wise training by BCGD for deep linear neural
networks. The learning rate is chosen to be (near) optimal according to (17). We emphasize
that the (near) optimal learning rate of (17) does not require any prior knowledge, and can
completely be determined by the loss function, the current weight matrices and the input
data matrix. This allows us to avoid a cumbersome grid-search over learning rate.

4.1 Random Data Experiments

Unless otherwise stated, we generate the input data matrix $X \in \mathbb{R}^{d_{in} \times m}$ whose entries
are i.i.d. samples from a Gaussian distribution $N(0, 1/n_0)$ and the output data matrix
$Y \in \mathbb{R}^{d_{out} \times m}$ whose entries are i.i.d. samples from a uniform distribution on $(-1, 2)$. The
number of training data is set to $m = 600$.

On the left of Figure 1, the approximation errors are plotted with respect to the number
of sweeps of the descending BCGD at different depths $L$. The input and output dimensions
are $d_{in} = n_0 = 128$ and $d_{out} = n_L = 10$, respectively. The width of the $\ell$-th layer is
$n_\ell = 128 = \max\{n_0, n_L\}$ and the orth-identity initialization (Section 2.3) is employed. We
see that the faster convergence is obtained as the depth grows. In an extreme case of the
depth $L = 400$, the global optimum is achieved by only after updating each weight
matrix once. These results are expected from Theorem 3. It is typical that the speed of
convergence is measured in terms of the number of updates of weight matrices, not the
amount of computation (Saxe et al., 2013; Arora et al. 2018b). However, to fairly compare
the effects of depth in the acceleration of convergence, the approximation errors need to
be plotted with respect to the number of iterations. On the right of Figure 1, the errors
are shown with respect to the number of iterations. We now see that training a depth 1 network multiple times results in the fastest decrease in the loss. This implies that in order for the faster convergence, it is better to train a depth 1 network \( L \) times than to train a depth \( L \) network once in this case. We remark that the condition number of the input data matrix was 2.6614. In this case, we do not have any advantages of using deep networks over a depth 1 network.

Figure 1: The approximation errors with respect to the number of (left) sweeps and (right) iterations of the descending BCGD with the optimal learning rate (11) at different depths \( L = 1, 10, 50, 100, 200, 400 \). The width is set to \( \max\{n_0, n_L\} = 128 \) and the orth-identity initialization is employed. When the depth is 400, the global optimum is achieved by after updating each weight matrix only once. However, when the errors are compared against the number of iterations, updating a single layer \( L \) times results in the faster loss decay than updating a \( L \) layer network once.

We now consider the input data matrix \( X \) whose condition number is rather big. To do this, we first generate \( X \) as in the above and conduct the singular value decomposition. We then assign randomly generated numbers from \( 10^{-5} + U(0, 1) \) to the singular values. In our experiment, the condition number of \( X \) was 236. The output data matrix \( Y \) is generated in the same way as before. In Figure 2, the approximation errors are plotted with respect to the number of (left) sweeps and (right) iterations of the descending BCGD at different depths \( L = 1, 3, 5, 7, 9, 11 \). When the speed of convergence is measured against the number of sweeps, we see that the deeper the network is, the faster the convergence is obtained. When the amount of computation is considered, unlike the case where \( X \) has a good condition number, we now see that the errors by deep linear networks decay drastically faster than those by a shallow network of depth 1. This demonstrates that over-parameterization by the depth can indeed accelerate convergence, even when the computational cost is considered. We note that from Theorem 2, the width plays no role in gradient-based training, as the width of intermediate layers is \( \max\{d_{\text{in}}, d_{\text{out}}\} \). Furthermore, the optimal learning rate is employed and adding more layers does not increase any representational power. Therefore,
this acceleration is solely contributed by the depth and this clearly demonstrates the benefit of using deep networks. We also observe that the error decrease per iteration does not grow proportionally to the depth. In this case, either depth 5 or 7 performs the best among others.

![Figure 2: The approximation errors with respect to the number of (left) sweeps and (right) iterations of the descending BCGD with the optimal learning rate (11) at different depths. The width is set to $\max\{n_0, n_L\} = 128$ and the orth-identity initialization is employed. The condition number of the input data matrix is 236. In terms of the number of sweeps, the deeper the network is, the faster convergence is obtained. In terms of the number of iterations (i.e., the computational cost is considered), unlike Figure 1 where $\text{cond}(X) \approx 2$, the use of deep networks drastically accelerates convergence of the loss when it is compared to those by a depth 1 network.](image)

Next, we show the ineffectiveness of training a network which has a layer whose width is less than $\max\{d_{\text{in}}, d_{\text{out}}\}$. Figure 3 shows the approximation errors with respect to the number of iterations of the descending BCGD. The input and output dimensions are $d_{\text{in}} = 128$ and $d_{\text{out}} = 20$, respectively. Two deep linear networks of depth $L = 100$ are compared. One has the architecture (Arch 1) of $n_\ell = 20$ for all $1 \leq \ell < L$. The other has the architecture (Arch 2) of $n_\ell = 128$ for all $1 \leq \ell < L$, but $n_{50} = 20$. Note that at the $k$-th iteration where $k = L - \ell + 1 \mod L$, the $(L - \ell + 1)$-th layer weight matrix is the only matrix updated. For the network of Arch 1, we see that the errors decrease mostly only after updating the first layer weight matrix. The errors before and after updating the first layer are marked as the circle symbols ($\circ$). For the network of Arch 2, we see that the errors decrease mostly after updating from the 50th to the 1st layer weight matrices. The errors before and after updating the 50th and the 1st layer matrices are marked as the asterisk symbols ($\ast$). These are expected from Theorem 3, as either $\sigma_{\min}(W_{k_{s,\ell-1}}^{(L:(i(\ell)+1))})$ or $\sigma_{\min}(W_{k_{s,\ell-1}}^{(k(\ell)-1):1}X)$ is zero, due to the network architecture. Precisely, the Arch 1 results in $\sigma_{\min}(W_{s,\ell-1}^{(L-\ell):1}X) = 0$, for all $s$ and $1 \leq \ell < L$, and the Arch 2 results in $\sigma_{\min}(W_{(L-\ell):1}^{s,\ell-1}X) =$
0 for all $s$ and $1 \leq \ell \leq 50$. For reference, the results by the network architecture (Arch 3) of $n_\ell = 128$ for all $\ell$ are shown as the dotted line. We see the fastest convergence by the network of Arch 3 among others. This demonstrates the ineffectiveness of training a deep linear network which has a layer whose width is less than $\max\{n_0, n_L\}$.

Figure 3: The approximation errors with respect to the number of iterations of the descending BCGD by three different network architectures. The results by the network of Arch 1 ($n_0 = 128, n_j = 20$) are shown as the dash line, those by the network of Arch 2 ($n_j = 128, n_{50} = n_L = 20$) are shown as the solid line, and those by the network of Arch 3 ($n_j = 128, n_L = 20$) are shown as the dotted line. This demonstrates the ineffectiveness of training a network which has a layer whose width is less than $\max\{n_0, n_L\}$.

We now compare the performance of layer-wise training by BCGD with two update orderings (top to bottom and bottom to top). Figure 4 shows the approximation errors with respect to the number of iterations of both the ascending and descending BCGD at three different initialization schemes (Section 2.3). We employ the DLNs of depth $L = 50$ and set the width of the $\ell$-th layer to $n_\ell = \max\{n_0, n_L\}$. On the left, the input and output dimensions are $d_{\text{in}} = 50$ and $d_{\text{out}} = 300$, respectively. It can be seen that for the orth-identity initialization, the errors by the ascending BCGD decay faster than those by the descending BCGD. For the balanced initialization, the opposite is observed. For the random initialization, the errors by both the ascending and descending orderings behave similarly. We see that the ascending BCGD with the orth-identity initialization results in the fastest convergence among others. On the right, the input and output dimensions are $d_{\text{in}} = 300$ and $d_{\text{out}} = 50$, respectively. It can be seen that for the balanced and the random initialization, the errors by the ascending BCGD decay faster than those by the descending BCGD. For the orth-identity initialization, the opposite is observed. In this case, the descending BCGD with the orth-identity initialization results in the fastest convergence among others. In all cases, we observe that the orth-identity initialization outperforms than other initialization schemes, regardless of the update ordering. Also, we found that when the orth-identity initialization is employed, the ascending BCGD performs better than the
descending BCGD if the output dimension is larger than the input dimension, and vice versa.

Figure 4: The approximation errors with respect to the number of iterations of both the ascending and descending BCGD by three different initialization schemes. The depth is $L = 50$ and the training is done over 600 data points. (Left) $n_0 = 50, n_j = 300$ for $0 < j \leq L$. (Right) $n_j = 300, n_L = 50$ for $0 \leq j < L$. When $n_0 = 50, n_j = 300$, the ascending BCGD with the orth-identity initialization results in the fastest convergence among others. When $n_j = 300, n_L = 50$, the descending BCGD with the orth-identity initialization results in the fastest convergence among others.

4.2 Real Data Experiments

We employ the dataset from UCI Machine Learning Repository's Gas Sensor Array Drift at Different Concentrations (Vergara et al., 2012; Rodriguez-Lujan et al., 2014). Specifically, we used the datasets Ethanol problem a scalar regression task with 2565 examples, each comprising 128 features (one of the largest numeric regression tasks in the repository). The input and output data sets are normalized to have zero mean and unit variance. After the normalization, the condition number of the input data matrix is 70,980. We note that this is the same data set used in (Arora et al., 2018b). The width of intermediate layers is set to $\max\{d_{\text{in}}, d_{\text{out}}\}$ and the identity initialization (Section 2.3) is employed. On the left of Figure 5, we show the errors by the descending BCGD with respect to the number of sweeps at five different depths $L = 1, 2, 3, 4, 5$. We use the optimal learning rate (11), which does not require any prior knowledge. It is clear that the errors by deep networks decay faster than those by a depth 1 network. In order to take the computational cost into account, on the right, we re-plot the figure with respect to the number of iterations. We clearly see that even considering the amount of computation, the over-parameterization by depth significantly accelerates convergence. We remark that in the work of (Arora et al., 2018b), although a different optimization method is used, the same problem is considered and the learning rate is chosen by a grid search. Similar implicit acceleration was demonstrated.
only for $L_4$-loss, not $L_2$-loss. In our experiment, by exploiting the layer-wise training and the optimal learning rate, we demonstrate implicit acceleration for $L_2$-loss even when the computational cost is considered. We remark that (Arora et al., 2018b) measured the speed of convergence in terms of the number of updates on each weight matrix, rather than the amount of computation (the computational cost for updating a depth 1 network $L$ times is comparable to those for updating a depth $L$ network once).

In Figure 6, we show the results by $L_4$-loss, i.e., $\frac{1}{m} \left[ \| W^{(k)} X - Y \|^4_{L_4} - \| W^* X - Y \|^4_{L_4} \right]$. The near optimal learning rate of (18) is employed. On the left and the right, the errors are plotted with respect to the number of sweeps and iterations, respectively. If the speed of convergence is measured in terms of the number of sweeps, i.e., the number of updates of each weight matrix, we see that the faster convergence is achieved by adding more layers. However, in terms of the number of iterations, i.e., when the amount of computation is considered, updating a single layer multiple-times results in the fastest error convergence than updating multiple layers once. For reference, we also plot the best error shown at (Arora et al., 2018b) after 1,000,000 iterations as the dashed line. We remark that when $L = 1$, the training procedure is identical to our setting and the only difference is in the selection of learning rate. It can be clearly seen that the (near) optimal learning rate results in a drastically faster loss decay than those by a grid search.

In Figure 5, we show the results by $L_2$-loss with respect to the number of (left) sweeps and (right) iterations. The network is trained over the UCI Machine Learning Repository’s dataset of 2565 examples. The condition number of $X$ is 70,980. The identity initialization is employed. The width is set to $n_\ell = 128$. In all depths, even the amount of computation is considered, the errors by deep linear networks decay faster than those by a single layer one.

We now train DLNs on the MNIST handwritten digit classification dataset. For an input image, its corresponding output vector contains a 1 in the index for the correct class and zeros elsewhere. The input and output dimensions are $d_{\text{in}} = 784$ and $d_{\text{out}} = 10$, respectively. In order to strictly compare the effect of depth, we employ the identity initialization to completely remove the randomness from the initialization. Also, we set.
Figure 6: The distances to the global optimum by $L_4$-loss with respect to the number of (left) sweeps and (right) iterations of the descending BCGD. The network is trained over the UCI Machine Learning Repository’s dataset of 2565 examples. The condition number of $X$ is 70,980. The identity initialization is employed. The width is set to $n_\ell = 128$. In terms of the number of sweeps, the deeper the network is, the faster the convergence is observed. However, when the amount of computation is considered, updating a depth 1 network $L$ times results in a faster loss decay than updating a depth $L$ network once.
the width to $784 = \max\{d_{in}, d_{out}\}$ according to Theorem 2. The networks are trained over the entire MNIST training dataset of 60,000 samples. The input data matrix $X$ is not full rank. Figure 7 shows the distances to the global optimum by $L_2$-loss with respect to the number of iterations of the descending BCGD at ten different depths $L = 1, \cdots, 10$. Thus, the speed of convergence is measured against the amount of computation. We observe the accelerated convergence by the network whose depth is even but not odd. We also see that the results by DLNs of odd-depth are very similar so that the lines are overlapping each other. In this case, the depth 2 network performs the best among others. We suspect that there is a connection between the parity of depth and the acceleration in convergence. We defer such further investigation to future work.

![Figure 7](image)

Figure 7: (to be viewed in color) The distances to the global optimum by $L_2$-loss with respect to the number of iterations of the descending BCGD. The identity initialization is employed. The network is trained over the MNIST training dataset of 60,000 samples. The width of intermediate layers is $n_L = 784$. The results by DLNs of odd-depth are very similar so that the lines are overlapping each other. The acceleration in convergence is observed by DLNs of even-depth.

5. Conclusion

In this paper, we studied a layer-wise training for deep linear networks using the block coordinate gradient descent (BCGD). We established a convergence analysis and found the optimal learning rate which results in the fastest decrease in the loss. More importantly, the optimal learning rate can directly be applied in practice as no prior knowledge is required. Also, we identified the effects of depth, width, and initialization in the training process. Firstly, we showed that when the orthogonal-like initialization is employed and the width of the intermediate layers is greater than or equal to both the input and output dimensions, the width plays no roles in gradient-based training. Secondly, under some assumptions, we proved that the deeper the network is, the faster the convergence is guaranteed. In an extreme case, the global optimum is achieved after updating each weight matrix only once.
Here, the speed of convergence is measured against the number of updates in each weight matrix, not the amount of computation. Thirdly, we empirically demonstrated that adding more layers could drastically accelerate convergence, when it is compared to those of a single layer, even when the computational cost is considered. Lastly, we establish a convergence analysis of the block coordinate stochastic gradient descent (BCSGD). Our analysis indicates that the BCSGD cannot reach the global optimum, however, the converged loss will be staying close to the global optimum. This can be understood as an implicit regularization, which avoids over-fitting, due to the stochasticity introduced by the random selection of mini-batch (of size 1). Numerical examples were provided to justify our theoretical findings and demonstrate the performance of the layer-wise training by BCGD.

Acknowledgments

The author would like to thank Dr. Pual Dupuis for his helpful discussion in the early stages of this work, Dr. Mark Ainsworth for his helpful comments and suggestions on both analysis and examples, and Dr. Nadav Cohen for sharing code for numerical experiments.
Appendix A. Proof of Theorem 2

Proof For a matrix $A$ of size $m \times n$ and a matrix $B$ of size $k \times s$ where $m \geq k, n \geq s$, we say $A$ is equivalent to $B$ up to zero-valued padding if

$$A = \begin{bmatrix} B & 0 \\ 0 & 0 \end{bmatrix},$$

and write $A \cong B$.

Lemma 9 Suppose $W_1^{k(1,\ell-1)} \cong \tilde{W}_1^{k(1,\ell-1)} \in \mathbb{R}^{\max\{n_0,n_L\} \times n_0}, W_L^{k(1,\ell-1)} \cong \tilde{W}_L^{k(1,\ell-1)} \in \mathbb{R}^{n_L \times \max\{n_0,n_L\}}$ and $W_j^{k(1,\ell-1)} \cong \tilde{W}_j^{k(1,\ell-1)} \in \mathbb{R}^{\max\{n_0,n_L\} \times \max\{n_0,n_L\}}$ for all $1 < j < L$.

Then,

$$W_{\ell}^{k(1,\ell)} \cong \tilde{W}_{\ell}^{k(1,\ell)} \in \begin{cases} \mathbb{R}^{\max\{n_0,n_L\} \times n_0}, & \text{if } \ell = 1, \\
\mathbb{R}^{\max\{n_0,n_L\} \times \max\{n_0,n_L\}}, & \text{if } 1 < \ell < L, \\
n_L \times \max\{n_0,n_L\}, & \text{if } \ell = L,
\end{cases}.$$

Proof Let $d_{\max} = \max\{n_0,n_L\}$. Note that if $W_1 \cong \tilde{W}_1 \in \mathbb{R}^{d_{\max} \times n_0}$, $W_L \cong \tilde{W}_L \in \mathbb{R}^{n_L \times d_{\max}}$, and $W_j \cong \tilde{W}_j \in \mathbb{R}^{d_{\max} \times d_{\max}}$ for $1 < j < L$, since $n_j \geq d_{\max}$ for $1 < j < L$, we have $W_{L:(j+1)} \cong \tilde{W}_{L:(j+1)}$ and $W_{(j-1):1} \cong \tilde{W}_{(j-1):1}$ for any $1 < j < L$. Specifically,

$$W_{L:(j+1)} = \begin{bmatrix} \tilde{W}_{L:(j+1)} & 0 \end{bmatrix}, \quad W_{(j-1):1} = \begin{bmatrix} \tilde{W}_{(j-1):1} \\ 0 \end{bmatrix}.$$ 

It then follows from the gradient descent update

$$W_{i(\ell)}^{k(s,\ell-1)} = W_{i(\ell)}^{k(s,\ell-1)} - \eta(W_{L:(i(\ell)+1)}^{k(s,\ell-1)})^T \Delta^{k(s,\ell-1)} X X^T (W_{L:(i(\ell)+1)}^{k(s,\ell-1)})^T,$$

where $i(\ell) = \ell$ if the ascending BCGD is employed and $i(\ell) = L - \ell + 1$ if the descending BCGD is employed, that we obtain

$$(W_{L:(i(\ell)+1)}^{k(s,\ell-1)})^T \Delta^{k(s,\ell-1)} X X^T (W_{L:(i(\ell)+1)}^{k(s,\ell-1)})^T \cong (\tilde{W}_{L:(i(\ell)+1)}^{k(s,\ell-1)})^T \Delta^{k(s,\ell-1)} X X^T (\tilde{W}_{L:(i(\ell)+1)}^{k(s,\ell-1)})^T \in \mathbb{R}^{d_{\max} \times d_{\max}}.$$

By the assumption on $W_j^{k(1,\ell-1)} \cong \tilde{W}_j^{k(1,\ell-1)}$, the proof is completed. \hfill \blacksquare

If the initial weight matrices satisfy

$$W_j^{(0)} \cong \tilde{W}_j^{(0)} \in \begin{cases} \mathbb{R}^{\max\{n_0,n_L\} \times n_0}, & \text{if } \ell = 1, \\
\mathbb{R}^{\max\{n_0,n_L\} \times \max\{n_0,n_L\}}, & \text{if } 1 < \ell < L, \\
n_L \times \max\{n_0,n_L\}, & \text{if } \ell = L,
\end{cases}$$

then
it follows from Lemma 9 that for any \( s \) and \( j \), there exists \( W_j^{(s)} \) such that
\[
W_j^{(s)} \approx \tilde{W}_j^{(s)} \in \begin{cases} \mathbb{R}^{\max\{n_0, n_L\} \times n_0}, & \text{if } \ell = 1, \\ \mathbb{R}^{\max\{n_0, n_L\} \times \max\{n_0, n_L\}}, & \text{if } 1 < \ell < L, \\ \mathbb{R}^{n_L \times \max\{n_0, n_L\}}, & \text{if } \ell = L, \end{cases}
\]
which completes the proof for the balanced initialization.

Suppose \( \min\{m, n\} > k = s \). We then write \( \mathbf{A} \approx_1 \mathbf{B} \) if \( \mathbf{A} \approx \tilde{\mathbf{B}} \) where \( \tilde{\mathbf{B}} \) is a square matrix of size \( \min\{m, n\} \) such that
\[
\tilde{\mathbf{B}} = \begin{bmatrix} \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{\min\{m, n\} - k} \end{bmatrix}.
\]

Let \( \mathbf{W}_j \) be a matrix of size \( n_j \times n_{j-1} \) and \( n_j \geq \max\{n_0, n_L\} \) for all \( 1 \leq j \leq L \). Suppose
\[
W_j \approx \tilde{W}_j \in \begin{cases} \mathbb{R}^{\max\{n_0, n_L\} \times n_0}, & \text{if } j = 1, \\ \mathbb{R}^{n_L \times \max\{n_0, n_L\}}, & \text{if } j = L, \end{cases} \quad (21)
\]

Let \( \mathbf{W}_L = [\tilde{W}_L \ 0] \), where \( \tilde{W}_L \in \mathbb{R}^{n_L \times \max\{n_0, n_L\}} \). Then,
\[
\mathbf{W}_{L:(j+1)} = [\tilde{W}_L \ 0] \begin{bmatrix} \tilde{\mathbf{B}}_{(L-1):(j+1)} & 0 \\ 0 & 0 \end{bmatrix}, \quad \tilde{\mathbf{B}}_{(L-1):(j+1)} = \begin{bmatrix} \tilde{\mathbf{W}}_{(L-1):(j+1)} & 0 \\ 0 & \mathbf{I}_{\min\{m, n\} - (j+1)}^{-1} \end{bmatrix},
\]
where \( n_{\min}(j) = \min_{1 \leq \ell \leq i} n_{\ell} \) for \( 1 \leq j \leq i + 1 \). Thus, \( \mathbf{W}_{L:(j+1)} \approx \tilde{\mathbf{W}}_{L:(j+1)} \). Similarly, \( \mathbf{W}_{(j-1):1} \approx \tilde{\mathbf{W}}_{(j-1):1} \). It then follows from a similar argument used in Lemma 9 that if the initial weight matrices satisfy (21), then the weight matrices updated by any gradient based optimization also satisfy (21). This completes the proof for the identity initialization. \( \blacksquare \)

**Appendix B. Proof of Theorem 3**

**Proof** For notational convenience, for \( j > i \), let
\[
W_j W_{j-1} \cdots W_i = W_{j:i}.
\]

By definition, it follows from the update rule that
\[
W_{\ell}^{(k+1)} = W_{\ell}^{(k)} - \eta_{\ell}^{k(\ell-1)} (W_{(\ell-1):1}^{(k+1)} \mathbf{X} J^{k(\ell-1)} W_{L:(\ell+1)}^{(k)})^T.
\]

By multiplying \( W_{(\ell-1):1}^{(k+1)} \mathbf{X} \) from right, and \( W_{L:(\ell+1)}^{(k)} \) from left and subtracting \( \mathbf{W}^* \mathbf{X} = \mathbf{Y} \mathbf{X}^\top \mathbf{X} \) in the both sides, we obtain
\[
(W_{L:(\ell+1)}^{(k+1)} W_{\ell:1}^{(k+1)} - W^*) \mathbf{X} = (W_{L:\ell}^{(k)} W_{(\ell-1):1}^{(k+1)} - W^*) \mathbf{X} - \eta_{\ell}^{k(\ell-1)} A_{\ell}^{(k)} (J_{k(\ell-1)})^T B_{\ell}^{(k+1)},
\]

24
where
\[ A^{(k)}_\ell = W^{(k)}_{L(\ell+1)}(W^{(k)}_{L(\ell+1)})^T \in \mathbb{R}^{d_{out} \times d_{out}}, \quad B^{(k)}_\ell = X^T(W^{(k)}_{(\ell-1):1})^T W^{(k)}_{(\ell-1):1} X \in \mathbb{R}^{m \times m}. \]

Since \( \ell(a; b) = (a - b)^2 / 2 \), we have
\[
X J^{(k, \ell-1)} = X(W^{(k)}_{L; \ell} W^{(k+1)}_{(\ell-1):1} X - Y)^T
\]
\[
= X(W^{(k)}_{L; \ell} W^{(k+1)}_{(\ell-1):1} X - YY^TX + YX^T X - Y)^T
\]
\[
= (W^{(k)}_{L; \ell} W^{(k+1)}_{(\ell-1):1} XX^T - YX^T X + Y(X^T XX^T - X^T))T
\]
\[
= ((W^{(k)}_{L; \ell} W^{(k+1)}_{(\ell-1):1} - W^*)XX^T)^T = X(\Delta^{k, \ell-1})^T,
\]
where \( X^T XX^T = (X^T X)^T X^T = (XX^T)^T = X^T \) is used in the 4th equality.

Let
\[ \Delta^{k, \ell} := W^{(k)}_{L(\ell+1)} W^{(k+1)}_{(\ell+1)} X - W^* X \in \mathbb{R}^{d_{out} \times m}. \]

Then we have
\[ \Delta^{k, \ell} = \Delta^{k, \ell-1} - \eta^{k, \ell-1}_\ell A^{(k)}_\ell \Delta^{k, \ell-1} B^{(k+1)}_\ell. \]

Since \( A^{(k)}_\ell \) and \( B^{(k)}_\ell \) are symmetric, we have diagonal transformations,
\[
(U^{(k)}_{\ell})^T A^{(k)}_{\ell} U^{(k)}_{\ell} = D^{(k)}_{A, \ell} = \text{diag}(\lambda^{(k)}_{\ell, i}), \quad 1 \leq i \leq d_{out},
\]
\[
(V^{(k)}_{\ell})^T B^{(k)}_{\ell} V^{(k)}_{\ell} = D^{(k)}_{B, \ell} = \text{diag}(\mu^{(k)}_{\ell, j}), \quad 1 \leq j \leq m,
\]
where \( V^{(k)}_{\ell} \) and \( U^{(k)}_{\ell} \) are orthogonal matrices, \( \lambda^{(k)}_{\ell, 1} \geq \cdots \geq \lambda^{(k)}_{\ell, d_{out}} \), and \( \mu^{(k)}_{\ell, 1} \geq \cdots \geq \mu^{(k)}_{\ell, m} \).

We remark that \( \mu^{(k)}_{\ell, d_{in}+1} = \cdots = \mu^{(k)}_{\ell, m} = 0 \) if \( d_{in} = n_0 < m \). Thus, we have
\[
\Delta^{k, \ell} = \Delta^{k, \ell-1} - \eta^{k, \ell-1}_\ell U^{(k)}_{\ell} D^{(k)}_{A, \ell}(U^{(k)}_{\ell})^T \Delta^{k, \ell-1} V^{(k+1)}_{\ell} D^{(k+1)}_{B, \ell}(V^{(k+1)}_{\ell})^T. \tag{23}
\]

Let \( \tilde{\Delta}^{k, \ell} = (U^{(k)}_{\ell})^T \Delta^{k, \ell} V^{(k+1)}_{\ell} \). Then, (23) becomes
\[
\tilde{\Delta}^{k, \ell} = \tilde{\Delta}^{k, \ell-1} - \eta^{k, \ell-1}_\ell D^{(k)}_{A, \ell} \tilde{\Delta}^{k, \ell-1} D^{(k+1)}_{B, \ell}.
\]

Then, the \((i, j)\)-entry of \( \tilde{\Delta}^{k, \ell} \) is
\[
(\tilde{\Delta}^{k, \ell})_{ij} = (1 - \eta^{k, \ell-1}_\ell \lambda^{(k)}_{\ell, i} \mu^{(k+1)}_{\ell, j})(\tilde{\Delta}^{k, \ell-1})_{ij}, \quad 1 \leq i \leq d_{out}, 1 \leq j \leq m,
\]
and we have
\[
\|\tilde{\Delta}^{k, \ell}\|_F^2 = \sum_{i, j} (1 - \eta^{k, \ell-1}_\ell \lambda^{(k)}_{\ell, i} \mu^{(k+1)}_{\ell, j})^2 (\tilde{\Delta}^{k, \ell-1})_{ij}^2 = \mathcal{F}(\eta^{k, \ell-1}_\ell).
\]
We then choose the learning rate which minimizes $F(\eta_{\ell}^{(k,\ell-1)})$ and it is

$$
\eta_{\text{opt}}^{(k,\ell-1)} = \frac{\sum_{i=1}^{\lambda_{\ell}^{(k,\ell-1)}} \left\| \frac{\partial L}{\partial W_{i,j}} \right\|_2^2}{\sum_{i=1}^{\lambda_{\ell}^{(k,\ell-1)}} W_{i,j}^4}.
$$

(24)

Thus, with the optimal learning rate of (24), we obtain

$$
\|\Delta^{(k,\ell)}\|_2^2 = \|\Delta^{(k,\ell-1)}\|_2^2 - \eta_{\text{opt}}^{(k,\ell-1)} \|\frac{\partial L}{\partial W_{i,j}}\|_2^2
$$

$$
= \|\Delta^{(k,\ell-1)}\|_2^2 - \left\| \frac{\partial L}{\partial W_{i,j}} \right\|_2^4 W_{i,j}^4.
$$

For a matrix $M$, the $j$-th column and the $i$-th row of $M$ are denoted by $(M)^{j}$ and $(M)^{i}$, respectively. We note that all rows of $\Delta^{(k,\ell-1)}$ are in \(\text{range}(X^T)\) and span\(\{(V^{(k+1)}_{\ell})^{j}; 1 \leq j \leq r_x\}\) = \(\text{range}(X^T)\), where $r_x = \text{rank}(X)$. We remark that if $\mu_{\ell,k}^{(k+1)} = 0$ for some $k \leq r_x$, we choose the corresponding $(V^{(k+1)}_{\ell})^{j}$ so that range$(X) = \text{span}\{(V^{(k+1)}_{\ell})^{j}; 1 \leq j \leq r_x\}$ holds. Thus, $(\Delta^{(k,\ell)} V^{(k+1)}_{\ell})^{j} = 0$ for $j > r_x$. This gives that the $(i,j)$-entry of $\tilde{\Delta}_{k,\ell}^{(k,\ell)}$ is equal to

$$
(\tilde{\Delta}_{k,\ell}^{(k,\ell)})_{ij} = \left(1 - \eta_{\ell}^{(k,\ell-1)} \lambda_{\ell,ij}^{(k+1)} \right) (\tilde{\Delta}_{k,\ell}^{(k,\ell-1)})_{ij}, \quad 1 \leq i \leq d_{\text{out}}, 1 \leq j \leq r_x,
$$

and zero otherwise.

Suppose that $(U^{(k)}_{\ell})^j \in K$ for all $1 \leq j \leq n_{L-1}$ where range$(Y X^\dagger) \subset K \subset \mathbb{R}^{n_L}$. It then can be checked that $(U^{(k)}_{\ell})^j \in K$ for all $k$ and $j$ and thus $(\Delta^{(k,\ell-1)})^{j} \in K$. Also, from the similar argument used in the above, we have

$$
\text{span}\{(U^{(k)}_{\ell})^{j}; j = 1, \ldots, r\} = K, \quad r = \dim K.
$$

Thus, $((U^{(k)}_{\ell})^T \Delta^{(k,\ell)})^i = 0$ for $i > r$ and we have

$$
(\tilde{\Delta}_{k,\ell}^{(k,\ell)})_{ij} = \left(1 - \eta_{\ell}^{(k,\ell-1)} \lambda_{\ell,ij}^{(k)} \mu_{\ell,ij}^{(k+1)} \right) (\tilde{\Delta}_{k,\ell}^{(k,\ell-1)})_{ij}, \quad 1 \leq i \leq r, 1 \leq j \leq r_x,
$$

(25)

and zero otherwise.

If the learning rate $\eta_{\ell}^{(k,\ell-1)}$ is chosen to satisfy

$$
0 < \eta_{\ell}^{(k,\ell-1)} < \frac{2}{\max_{ij} \left(\lambda_{\ell,ij}^{(k+1)} \mu_{\ell,ij}^{(k)}\right)} = \frac{2}{\sigma_{\max}^{2}(W^{(k,\ell-1)}_{\ell}+1) \sigma_{\max}^{2}(W^{(k,\ell-1)}_{\ell}+1) X},
$$

we have

$$
((\tilde{\Delta}_{k,\ell}^{(k,\ell)})^{2} \leq ((\tilde{\Delta}_{k,\ell}^{(k,\ell-1)})^{2} (\gamma^{(k,\ell-1)})^{2},
$$

26
where \( \gamma^{(k,\ell-1)} = \max\{\gamma_1^{(k,\ell-1)}, \gamma_2^{(k,\ell-1)}\} \),

\[
\gamma_1^{(k,\ell-1)} = 1 - \eta^{k,s(\ell-1)} \sigma_2(W_{L_i((\ell)-1)} W_{(i(\ell)-1):1} X), \\
\gamma_2^{(k,\ell-1)} = \eta^{k,s(\ell-1)} \|W^{(k,s(\ell-1))}_{L_i((\ell)-1)}\|_F^2 \|W^{(k,s(\ell-1))}_{(i(\ell)-1):1} X\|_F^2 - 1.
\]

Note that from the relation of \( \|M\|_F^2 = \text{Tr}(MM^T) \), we have

\[
\|\tilde{\Delta}^{(k,\ell)}\|_F^2 = \text{Tr}((U^{(k)}_\ell)^T \Delta^{(k,\ell)} \tilde{V}_{k,\ell}(\tilde{V}_{k,\ell})^T (\Delta^{(k,\ell)} \eta^{(k,\ell)})^T U^{(k)}_\ell) = \text{Tr}((U^{(k)}_\ell)^T \Delta^{(k,\ell)} (\Delta^{(k,\ell)} \eta^{(k,\ell)})^T U^{(k)}_\ell)
\]

\[
= \text{Tr}(\Delta^{(k,\ell)} (\Delta^{(k,\ell)} \eta^{(k,\ell)})^T U^{(k)}_\ell (U^{(k)}_\ell)^T) = \text{Tr}(\Delta^{(k,\ell)} (\Delta^{(k,\ell)} \eta^{(k,\ell)})^T) = \|\Delta^{(k,\ell)}\|_F^2.
\]

Therefore,

\[
\|\tilde{\Delta}^{(k,\ell)}\|_F^2 \leq \|\tilde{\Delta}^{(k,\ell-1)}\|_F^2 (\gamma^{(k,\ell-1)})^2 \iff \|\Delta^{(k,\ell)}\|_F^2 \leq \|\Delta^{(k,\ell-1)}\|_F^2 (\gamma^{(k,\ell-1)})^2.
\]

By recursively applying the above, we obtain

\[
\|\Delta^{(k,\ell)}\|_F^2 \leq \|\Delta^{(k,0)}\|_F^2 \prod_{s=0}^{k-1} \left( \prod_{\ell=1}^L (\gamma^{(k,s,\ell-1)})^2 \right),
\]

which completes the proof.

\[\blacksquare\]

Appendix C. Proof of Lemma 5

**Proof** Suppose \( \|W^{(k)} - W^*\|_F \leq \tilde{\sigma}_{\min} - c/\|X\| \) where \( \tilde{\sigma}_{\min} = \sigma_{\min}(W^* X)/\|X\| \), where \( c \) will be chosen later. It then follows from the assumption that

\[
\|W^{(k)} X - W^* X\|_F \leq \|W^{(k)} - W^*\|_F \|X\| \leq \sigma_{\min}(W^* X) - c.
\]

Then for any \( W \) satisfying \( \|W X - W^* X\|_F \leq \|W^{(k)} X - W^* X\|_F \), we have

\[
\sigma_{\min}(W X) \geq \sigma_{\min}(W^* X) - \sigma_{\max}(W X - W^* X) \geq \sigma_{\min}(W^* X) - \|W X - W^* X\|_F \geq c > 0.
\]

From Theorem 3, since \( \|W^{(k)} X - W^* X\|_F \leq \|W^{(k)} X - W^* X\|_F \) for any \( j \), we obtain

\[
\sigma_{\min}(W^{(k)} X) \geq c > 0.
\]

For notational convenience, let \( A = W^{(k)}_{L_i((\ell)-1)} \), \( B = W^{(k)}_{i(\ell)-1} \), and \( C = W^{(k)}_{(i(\ell)-1):1} X \).

Then, \( W^{(k,\ell-1)} X = ABC \). Note that \( \sigma_s(ABC) = \sigma_s(C^T B^T A^T) \). It then follows from

\[
0 < c \leq \sigma_{\min}(ABC) \leq \sigma_s(ABC) = \max_{S: \dim(S) = s} \min_{x \in S, \|x\| = 1} \|ABCx\| \\
\leq \|AB\| \max_{S: \dim(S) = s} \min_{x \in S, \|x\| = 1} \|Cx\| \quad (27)
\]

\[
= \|AB\| \sigma_s(C), \quad \min\{n_0, n_L\} \leq s \leq 1,
\]

that \( \sigma_s(C) > \frac{c}{\|AB\|} \). Similarly, \( \sigma_s(A) > \frac{c}{\|BC\|} \).
Note that it follows from Theorem 2 that for any $s$ and $\ell$,

$$
W^{(s)}_j \approx \tilde{W}^{(s)}_j \in \begin{cases}
\mathbb{R}^{\max\{n_0, n_L\} \times n_0}, & \text{if } j = 1, \\
\mathbb{R}^{n_L \times \max\{n_0, n_L\}}, & \text{if } j = L,
\end{cases}
$$

and

$$
W^{(s)}_j \approx \tilde{W}^{(s)}_j \in \mathbb{R}^{\max\{n_0, n_L\} \times \max\{n_0, n_L\}}, \text{ if } 1 < j < L.
$$

(28)

Then, for any $k = (k_1, \ldots, k_L)$ and $\ell \in \{1, \ldots, L - 1\}$, we have

$$
W^{k}_{\ell; \ell+1} = \tilde{W}^{(k_L)}_{\ell} \cdots \tilde{W}^{(k_{\ell+1})}_{\ell+1}, \quad W^{k}_{\ell+1; 1} X = \tilde{W}^{(k_{\ell-1})}_{\ell} \cdots \tilde{W}^{(k_1)}_1 X.
$$

Since $n_\ell \geq \max\{n_0, n_L\}$, we have

$$
\sigma_{\min}(W^{k}_{L:(i(\ell))}) \geq \prod_{j=i(\ell)+1}^{L} \sigma_{\min}(\tilde{W}^{(s)}_{j}).
$$

\[ \text{Similarly, } \sigma_{\min}(W^{k}_{(i(\ell)-1):1}) \geq \sigma_{\min}(X) \prod_{j=1}^{(i(\ell)-1)-1} \sigma_{\min}(\tilde{W}^{(s)}_{j}). \] From (27), we have

$$
\|W^{k}_{L:(i(\ell))}\| \geq \sigma_s(W^{k}_{L:(i(\ell))}) \geq \frac{c}{\|W^{(0)}_{i(j)}\|},
$$

and

$$
\|W^{k}_{(i(\ell)-1):1}\| \geq \sigma_s(W^{k}_{(i(\ell)-1):1}) \geq \frac{c}{\|W^{(0)}_{L:(i(\ell)+1)}\|}.
$$

(29)

Let

$$
\mathcal{R}(\theta^{k}_{s, \ell}) = \max_{1 \leq j \leq \ell} \|W^{k}_{i(j)} - W^{(0)}_{i(j)}\|,
$$

(30)

and

$$
\mathcal{R}(sL + \ell) = \max \left\{ \max_{0 \leq i < s} \mathcal{R}(\theta^{k}_{i, L}) , \mathcal{R}(\theta^{k}_{s, \ell}) \right\}.
$$

(31)

By applying the induction on the number of iterations of the BCGD, we claim that there exists $0 < R < 1$ such that

$$
\mathcal{R}(k) \leq R, \forall k.
$$

Since $\mathcal{R}(0) = 0$, the base case holds trivially. Suppose $\mathcal{R}(sL + \ell - 1) \leq R$. We want to show that $\mathcal{R}(sL + \ell) \leq R$. Note that since $W^{k}_{i(j)} = W^{k}_{i(j)}$ for $j \neq \ell$, it suffices to consider $W^{k}_{i(\ell)}$. Suppose the learning rates satisfy (9). It follows from the BCGD updates

$$
W^{k}_{i(\ell)} = W^{k}_{i(\ell)} - \eta_{\ell} (W^{k}_{L:(i(\ell)+1)})^T \Delta^{k}_{(\ell-1)} (W^{k}_{(i(\ell)-1):1} X)^T,
$$

that

$$
\|W^{k}_{i(\ell)} - W^{(0)}_{i(\ell)}\| \leq \|W^{k}_{i(\ell)} - W^{(0)}_{i(\ell)}\| + \eta_{\ell} \|\Delta^{k}_{(\ell-1)}\| \|W^{k}_{(i(\ell)-1):1} X\| \Delta^{k}_{(\ell-1)}
$$

$$
\leq \|W^{k}_{i(\ell)} - W^{(0)}_{i(\ell)}\| + \frac{\eta_{\ell} \|\Delta^{k}_{(\ell-1)}\|}{\|W^{k}_{L:(i(\ell)+1)}\| \|W^{k}_{(i(\ell)-1):1} X\|}.
$$

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Using (29), we obtain

$$\|W_{i(\ell)}^{k(s, \ell)} - W_{i(\ell)}^{(0)}\| \leq \|W_{i(\ell)}^{k(s, \ell - 1)} - W_{i(\ell)}^{(0)}\| + \eta \frac{\|W_{L:1}^{k(s, \ell - 1)} X \| \Delta_{L:1}^{k(s, \ell - 1)}\|_F}{c^2}. \tag{32}$$

Also, note that by the induction hypothesis and (28), we have $\sigma_{\max}(W_j^{k(s, \ell - 1)}) < 1 + R$ and

$$R > \|W_j^{k(s, \ell - 1)} - W_j^{(0)}\| \geq \|(W_j^{k(s, \ell - 1)} - W_j^{(0)})z\| \geq \|W_j^{(0)}z\| - \|W_j^{k(s, \ell - 1)}z\| = 1 - \sigma_{\min}(W_j^{k(s, \ell - 1)}) \implies \sigma_{\min}(W_j^{k(s, \ell - 1)}) > 1 - R,$$

where $\|z\| = 1$. Here, we set $z$ to be the right singular vector of $W_j^{k(s, \ell - 1)}$ which corresponds to $\sigma_{\min}(\tilde{W}_j^{k(s, \ell - 1)})$. Then, $z$ has zero-values from $(\max\{n_0, n_L\} + 1)$-th to $n_{j-1}$-th entries. Recall that $W_j^{(0)}$ is equivalent to an orthogonal matrix upto zero-valued padding. This allows us to conclude $\|W_j^{(0)}z\| = 1$, which makes the fourth equality of (33) hold. Thus, we have

$$\sigma_{\min}(W_j^{k(s, \ell - 1)})\sigma_{\min}(W_{\ell:1}^{k(s, \ell - 1)}) \geq \sigma_{\min}(X)(1 - R)^{L-1},$$

$$\sigma_{\max}(W_j^{k(s, \ell - 1)})\sigma_{\max}(W_{\ell:1}^{k(s, \ell - 1)}) \leq \sigma_{\max}(X)(1 + R)^{L-1}.$$  

It then follows from (10) that

$$\gamma_{k,j-1}^k = 1 - \frac{\eta}{\kappa^2(W_j^{k(s, \ell - 1)})\kappa^2(W_{\ell:1}^{k(s, \ell - 1)})X} < \gamma := 1 - \frac{\eta}{\kappa^2(X)} \frac{1 - R}{1 + R}^{2(L-1)}, \tag{34}$$

for $0 \leq k < s$ with $1 \leq j \leq L$ and $k = s$ with $1 \leq j < \ell$. From (32), (34) and Theorem 3, we obtain

$$\|W_{i(\ell)}^{(s+1)} - W_{i(\ell)}^{(0)}\| \leq \|W_{i(\ell)}^{(s)} - W_{i(\ell)}^{(0)}\| + \frac{\eta(1 + R)^{L+1}}{c^2} \|X\| \|\Delta_0\|_F \gamma^{s+L-1}. \tag{35}$$

The recursive relation with respect to $s$ gives

$$\|W_{i(\ell)}^{(s+1)} - W_{i(\ell)}^{(0)}\| \leq \sum_{t=0}^{s} \frac{(1 + R)^{L+1}}{c^2} \eta \|X\| \|\Delta_0\|_F \gamma^{t+L-1} \leq \frac{(1 + R)^{L+1}}{c^2} \eta \|X\| \|\Delta_0\|_F \frac{1}{1 - \gamma^L} \leq \frac{(1 + R)^{L+1}}{c^2} \eta \|X\| \|\Delta_0\|_F \frac{1}{L \kappa_\gamma^2(X)} \frac{(1 - R)}{(1 + R)}^{2(L-1)} \leq \|X\|^2 \|W_0 - W^*\|_F R^2(X) \frac{(1 + R)^{L+1}}{c^2} \frac{1}{L \left(\frac{1 - R}{1 + R}\right)^{2(L-1)}}.$$  

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Let \( \tilde{c} = c/\|X\| \). If \( R = R_L := \frac{(5L-3)-\sqrt{(5L-3)^2-4L}}{2L} \) and
\[
\tilde{c} \geq \kappa^2(X) \left( -1 + \sqrt{1 + 4h(L)\tilde{\sigma}_{\min}/\kappa^2(X)} \right) / 2h(L),
\]
(35)
where \( h(L) = \frac{LR_L(1-R_L)^2L^{-2}}{(1+R_L)^{3L-1}} \), we have
\[
\|W^{(s+1)}_{\ell(t)} - W^{(0)}_{\ell(t)}\| \leq \frac{\|W^k - W^*\|_F}{\tilde{c}} \frac{\|X\|}{\kappa^2(X)} \left( \frac{1+R}{\frac{1-R}{1+R}} \right)^{2(L-1)} \leq R.
\]
This can be checked as follows. First, we note that the maximum of \( x^{(1+x)^2} \) where \( 0 < x < 1 \) is obtained at \( x = R_L \). It also follows from the assumption of \( \|W^k - W^*\|_F \leq \tilde{\sigma}_{\min} - \tilde{c} \) that
\[
\tilde{c} \geq \kappa^2(X) \left( -1 + \sqrt{1 + 4h(L)\tilde{\sigma}_{\min}/\kappa^2(X)} \right) / 2h(L)
\]
\[
\iff \quad \frac{2h(L)}{\kappa^2(X)} \tilde{c} + 1 \geq \sqrt{1 + 4h(L)\tilde{\sigma}_{\min}/\kappa^2(X)}
\]
\[
\iff \quad \frac{(\tilde{\sigma}_{\min} - \tilde{c})\kappa^2(X)}{\tilde{c}^2} \leq h(L) = LR \left( \frac{1-R}{1+R} \right)^{2(L-1)}
\]
\[
\iff \quad \|W^k - W^*\|_F \kappa^2(X) \leq LR \left( \frac{1-R}{1+R} \right)^{2(L-1)}
\]
\[
\iff \quad \|W^k - W^*\|_F \kappa^2(X) \leq LR \left( \frac{1-R}{1+R} \right)^{2(L-1)} \quad \iff \quad \|W^k - W^*\|_F \kappa^2(X) \leq \frac{L}{\left( \frac{1-R}{1+R} \right)^{2(L-1)}} \leq R.
\]
Hence, \( \|W^{(s+1)}_{\ell(t)} - W^{(0)}_{\ell(t)}\| < R. \) Thus, by induction, we conclude that \( R(k) < R \) for all \( k \).

By letting \( \tilde{c} = \kappa^2(X) \left( -1 + \sqrt{1 + 4h(L)\tilde{\sigma}_{\min}/\kappa^2(X)} \right) / 2h(L) \), the assumption on \( \|W^k - W^*\|_F \) becomes
\[
\|W^k - W^*\|_F \leq \tilde{\sigma}_{\min} - \kappa^2(X) \left( -1 + \sqrt{1 + 4h(L)\tilde{\sigma}_{\min}/\kappa^2(X)} \right) / 2h(L)
\]
\[
= \frac{1}{2h(L)} \left( 2h(L)\tilde{\sigma}_{\min} + \kappa^2(X) - \kappa(X)\sqrt{\kappa^2(X) + 4h(L)\tilde{\sigma}_{\min}} \right)
\]
\[
= \frac{1}{2h(L)} \left( 2h(L)\tilde{\sigma}_{\min} + \kappa^2(X) \right)^2 - \kappa^2(X) \kappa(X)\sqrt{\kappa^2(X) + 4h(L)\tilde{\sigma}_{\min}}
\]
\[
= \frac{2h(L)\tilde{\sigma}_{\min} + \kappa^2(X)}{2h(L)\tilde{\sigma}_{\min} + \kappa^2(X)} \left( 1 + \sqrt{1 + 4h(L)\tilde{\sigma}_{\min}/\kappa^2(X)} \right)
\]
\[
= \frac{\tilde{\sigma}_{\min}}{1 + \kappa^2(X) \left( \frac{1+\sqrt{1+4h(L)\tilde{\sigma}_{\min}/\kappa^2(X)}}{2h(L)\tilde{\sigma}_{\min}} \right)}.
\]
Therefore, under the above assumption on \(\|W^{k_0} - W^*\|_F\), we have
\[
\gamma_{k(\ell-1)} < \gamma_L := 1 - \frac{\eta}{\kappa^2(X)} \left(1 - \frac{R_L}{1 + R_L}\right)^{2(L-1)}.
\]

Furthermore, it follows from
\[
LR_L = \frac{5L - 3}{2} \left(1 - \sqrt{1 - \frac{4L}{(5L - 3)^2}}\right) = \frac{2L}{5L - 3} = \frac{2}{5} \frac{1}{L} \cdot \frac{1}{1 + \sqrt{1 - \frac{4L}{(5L - 3)^2}}},
\]
that \(\lim_{L \to \infty} LR_L = \frac{1}{5}\) and \(\lim_{L \to \infty} R_L = 0\). Also, since \(LR_L\) and \(R_L\) are decreasing functions of \(L\), we have
\[
\left(1 - \frac{R_L}{1 + R_L}\right)^{2(L-1)} \geq \left(1 - \frac{2R_L}{1 + R_L}\right)^{2L} \geq 1 - \frac{4LR_L}{1 + R_L} \geq \frac{1}{5}.
\]
Hence, we can conclude that
\[
\gamma_L = 1 - \frac{\eta}{\kappa^2(X)} \frac{4LR_L}{1 + R_L} \leq \gamma = 1 - \frac{\eta}{5\kappa^2(X)},
\]
which completes the proof. \(\blacksquare\)

Appendix D. Proof of Theorem 6

**Proof** Since \(n_\ell \geq \max\{n_0, n_L\}\) and the initial weight matrices are from the orth-identity initialization (Section 2.3), it follows from Theorem 2 that \(W^{(0)}_{(\ell-1):1} \approx W^{(0)}_{(\ell-1):1} \in \mathbb{R}^{\max\{n_0, n_L\} \times n_0}\) and \((W^{(0)}_{(\ell-1):1})^T W^{(0)}_{(\ell-1):1} = I_{n_0}\). Thus,
\[
\sigma_{\max}(W^{(0)}_{(\ell-1):1}) = 1 = \sigma_{\min}(W^{(0)}_{(\ell-1):1}).
\]
Note that since \(X\) is a full row-rank matrix, \(XX^T\) is invertible. In what follows, we will show that \(\|W^{(1)}_{L:(L-\ell+1)}\| = 0\) if
\[
W^* = YX^\dagger = W^{k(0,\ell-1)}(I_{n_0} - \|X\|^2(XX^T)^{-1}/\eta). \tag{36}
\]
Suppose \(W^*\) does not satisfy the condition of (36) for all \(\ell\). For \(\ell = 1\), we have \(\eta_{1}^{k(0,0)} = \eta/\|X\|^2\) since \((W^{(0)}_{(L-1):1})^T W^{(0)}_{(L-1):1} = I_{n_0}\). Suppose \(W^{(1)}_{L} = 0\) and let \(\Delta^{k(0,\ell-1)} = W^{k(0,\ell-1)} - W^*\). Then,
\[
0 = W^{(1)}_{L} = W^{(0)}_{L} - \eta_{1}^{k(0,0)}(W^{(0)}_{(L-1):1})^T XX^T(\Delta^{k(0,0)})(W^{(0)}_{(L-1):1})^T,
\]
\[
W^{(0)}_{L} = \eta_{1}^{k(0,0)} \Delta^{k(0,0)} XX^T(W^{(0)}_{(L-1):1})^T,
\]
\[
W^{k(0,0)} = \eta_{1}^{k(0,0)}(W^{k(0,0)} - W^*) XX^T(W^{(0)}_{(L-1):1})^T W^{(0)}_{(L-1):1},
\]
\[
W^* = W^{k(0,0)}(I_{n_0} - (\eta_{1}^{k(0,0)} XX^T)^{-1}).
\]
which contradicts to the assumption of $W^*$ being not satisfying (36). Hence, $W_L^{(1)} \neq 0$.

Now, suppose $\|W_{L:(L-\ell+2)}\| \neq 0$ and we want to show $\|W_{L:(L-\ell+1)}^{(1)}\| \neq 0$. Suppose not, i.e, $W_{L:(L-\ell+1)}^{(1)} = 0$. Then, we have

$$W_{L:(L-\ell+1)}^{(1)} = W_{L:(L-\ell+2)}^{(0)} - \eta L \ell k_{(0,\ell-1)} W_{L:(L-\ell+2)}^{(0)} X X^T (\Delta W_{L:(L-\ell+2)}^{(0,\ell-1)})^T,$$

which contradicts to the assumption of $W^*$. Hence, $W_{L:(L-\ell+1)}^{(1)} \neq 0$. By induction, we conclude that $W_{L:(L-\ell+1)}^{(1)} \neq 0$ for all $\ell$. Thus, it follows from Theorem 3 that

$$\|W^{k_1} X - W^* X\|_F < \|W^{k_0} X - W^* X\|_F \left(1 - \frac{\eta}{\kappa^2(X)}\right)^{L}. \quad (37)$$

Since $L$ is chosen to satisfy

$$\|W^{k_1} X - W^* X\|_F \leq \|W^{k_0} X - W^* X\|_F \left(1 - \frac{\eta}{\kappa^2(X)}\right)^{L} \leq \frac{\sigma_{\min}(W^* X)}{c},$$

where $c$ is defined in (13), it follows from Lemma 5 and Theorem 4 that $\|W^{(j)}_{L:j}\| \neq 0$ for all $j$ and $s$, and

$$\|W^{k_s} X - W^* X\|_F \leq \|W^{k_1} X - W^* X\|_F (\gamma^{L-1})^{s-1} \left(1 - \frac{\eta}{\kappa^2(X)}\right)^{s-1}.$$

Note that $\left(1 - \frac{1}{\kappa^2(X)}\right)^{s-1}$ is from the fact that $\|W^{(s)}_{L:s}\| \neq 0$ for all $1 \leq s$. Hence, we have

$$\|W^{k_s} X - W^* X\|_F \leq \|W^{k_0} X - W^* X\|_F (\gamma^{L-1})^{s-1} \left(1 - \frac{\eta}{\kappa^2(X)}\right)^{L+s-1},$$

and the proof is completed.

**Appendix E. Proof of Theorem 7**

**Proof** For notational convenience, let $\ell(z) = \ell(z;b)$. Since $\ell(\cdot)$ is convex, differentiable and $|\ell'(z) - \ell'(x)| \leq C_{\text{Lip}} |z - x|$, we have

$$\ell(z) \leq \ell(x) + \ell'(x)(z - x) + \frac{1}{2} \ell''(x)(z - x)^2 \leq \ell(x) + \ell'(x)(z - x) + \frac{C_{\text{Lip}}}{2} (z - x)^2.$$
Let $W^{k(k,\ell)} = W_{L:(L-\ell+1)}^{(k+1)} W_{(L-\ell+1):1}^{(k)}$, $\hat{y}^{i}_{(k,\ell)} = W^{k(k,\ell)} x^i$ and $\hat{Y}^{(k,\ell)} = [\hat{y}^{1}_{(k,\ell)}, \cdots, \hat{y}^{m}_{(k,\ell)}] = W^{k(k,\ell)} X$. Then, we have

$$\ell((\hat{y}^{i}_{(k,\ell)})_j; y^j_j) \leq \ell((\hat{y}^{i}_{(k,\ell-1)})_j; y^j_j) + \ell((\hat{y}^{i}_{(k,\ell-1)})_j; (y^i_{(k,\ell-1)})_j - (\hat{y}^{i}_{(k,\ell-1)})_j) + \frac{C_{\text{Lip}}}{2} ((\hat{y}^{i}_{(k,\ell)})_j - (\hat{y}^{i}_{(k,\ell-1)})_j)^2.$$  

(38)

For notational convenience, for $j > i$, let

$$W_j W_{j-1} \cdots W_i = W_{j:i}.$$  

It follows from the BCGD update rule that

$$W^{(k+1)}_{L:(L+1)} W^{(k)}_{(L-\ell+1):1} = W^{(k)}_{L:(L-\ell+1)} - \eta^{k(k,\ell-1)}_{\ell} (W^{(k)}_{(L-\ell+1):1} X J^{k(k,\ell-1)} W^{(k+1)}_{L:(L-\ell+2)})) T.$$  

By multiplying $W^{(k)}_{(L-\ell+1):1} X$ from right, and $W^{(k+1)}_{L:(L-\ell+2)}$ from left in the both sides, we obtain

$$W^{(k+1)}_{L:(L-\ell+1)} W^{(k)}_{(L-\ell+1):1} X = W^{(k+1)}_{L:(L-\ell+2)} W^{(k)}_{(L-\ell+1):1} X - \eta^{k(k,\ell-1)}_{\ell} (J^{k(k,\ell-1)})^T C^{(k)}_{\ell},$$  

where

$$A^{(k)}_{\ell} = W^{(k)}_{(L-\ell+2):1} (W^{(k)}_{(L-\ell+2):1})^T \in \mathbb{R}^{d_{\text{out}} \times d_{\text{out}}}, \quad B^{(k)}_{\ell} = (W^{(k)}_{(L-\ell+1):1} X)^T W^{(k)}_{(L-\ell+1):1} X \in \mathbb{R}^{m \times m}.$$  

Thus, we have

$$\hat{Y}_{(k,\ell)} - \hat{Y}^{(k,\ell-1)} = (W^{k(k,\ell)} - W^{k(k,\ell-1)}) X = -\eta^{k(k,\ell-1)}_{\ell} A^{(k)}_{\ell} (J^{k(k,\ell-1)})^T B^{(k+1)}_{\ell},$$  

where $\hat{Y}_{(k,\ell)} = W^{k(k,\ell)} X$. Let

$$\eta^{k(k,\ell-1)}_{\ell} = \max \left( \frac{\sigma_{\text{max}}(W^{(k+1)}_{L:(L-\ell+2)}) \sigma_{\text{max}}(W^{(k)}_{(L-\ell+1):1} X)}{\sigma_{\text{max}}(W^{(k)}_{(L-\ell+1):1} X)} \right).$$  

Also, let $\Delta^{k(k,\ell)} = \mathcal{L}(\theta^{k(k,\ell)}) - \mathcal{L}(\theta^*)$, $\Delta^{k(k,\ell)} = (W^{k(k,\ell-1)} - W^*) X$, and

$$J^{k(k,\ell-1)} = (W^{(k+1)}_{L:(L-\ell+1):1}) X J^{k(k,\ell-1)} W^{(k+1)}_{L:(L-\ell+2)} X = A^{(k+1)}_{\ell} (J^{k(k,\ell-1)})^T B^{(k+1)}_{\ell},$$  

Let $\mathcal{L}(\hat{Y}_{(k,\ell)}) = \mathcal{L}(\theta^{k(k,\ell)})$. By combining it with (38),

$$\mathcal{L}(\hat{Y}_{(k,\ell)}) \leq \mathcal{L}(\hat{Y}_{(k,\ell-1)}) - \eta^{k(k,\ell-1)}_{\ell} ((J^{k(k,\ell-1)})^T A^{(k+1)}_{\ell} (J^{k(k,\ell-1)})^T B^{(k+1)}_{\ell} F) + \frac{C_{\text{Lip}}}{2} ((\eta^{k(k,\ell-1)}_{\ell})^2 \|A^{(k+1)}_{\ell} (J^{k(k,\ell-1)})^T B^{(k+1)}_{\ell}\|_F^2.$$  

$$= \mathcal{L}(\hat{Y}_{(k,\ell-1)}) - \eta^{k(k,\ell-1)}_{\ell} \|J^{k(k,\ell-1)}\|_F^2 + \frac{C_{\text{Lip}}}{2} ((\eta^{k(k,\ell-1)}_{\ell})^2 \|A^{(k+1)}_{\ell} (J^{k(k,\ell-1)})^T B^{(k+1)}_{\ell}\|_F^2.$$  

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It then can be checked that the learning rate which minimizes the above upper bound is
\[
\eta_{\text{opt}}^{(k,\ell-1)} = \frac{\|J^{(k,\ell-1)}\|^2_F}{C_{\text{Lip}}\|W_{L:(\ell-1)}^{(k+1)}J^{(k,\ell-1)}W^{(k)}_{(\ell-1):1}X\|^2_F}.
\]

(39)

Also, it follows from
\[
\|J^{(k,\ell-1)}\|^2_F \leq C_{\text{Lip}}\|W_{L:(\ell-1)}^{(k+1)}\|^2\|J^{(k,\ell-1)}\|^2_F = \mu_{\max}^{(k,\ell-1)}\|J^{(k,\ell-1)}\|^2_F
\]

that
\[
L(\hat{Y}_{(k,\ell-1)}) \leq L(\hat{Y}_{(k,\ell-1)}) - \eta^{k(k,\ell-1)}_\ell \|J^{k(k,\ell-1)}\|^2_F + \frac{C_{\text{Lip}}}{2} \|\eta^{k(k,\ell-1)}_\ell\|^2 A^{(k+1)}(J^{(k,\ell-1)})^T D^{(k)}_\ell \|J^{(k,\ell-1)}\|^2_F
\]
\[
\leq L(\hat{Y}_{(k,\ell-1)}) - \eta^{k(k,\ell-1)}_\ell \|J^{k(k,\ell-1)}\|^2_F + \frac{C_{\text{Lip}}}{2} \|\eta^{k(k,\ell-1)}_\ell\|^2 \mu_{\max}^{(k,\ell-1)}\|J^{(k,\ell-1)}\|^2_F
\]
\[
= L(\hat{Y}_{(k,\ell-1)}) - (1 - \frac{C_{\text{Lip}}}{2} \eta^{k(k,\ell-1)}_\ell \mu_{\max}^{(k,\ell-1)}\|J^{(k,\ell-1)}\|^2_F.
\]

If \(0 < \eta^{k(k,\ell-1)}_\ell < \frac{2}{C_{\text{Lip}}\mu_{\max}^{(k,\ell-1)}},\) unless \(\|J^{(k,\ell-1)}\|_F = 0,\) the loss function is strictly decreasing.

Suppose \(0 < \eta^{k(k,\ell-1)}_\ell \leq \frac{1}{C_{\text{Lip}}\mu_{\max}^{(k,\ell-1)}}.\) Then, since \(-1 - \frac{C_{\text{Lip}}}{2} \eta^{k(k,\ell-1)}_\ell \mu_{\max}^{(k,\ell-1)}\|J^{(k,\ell-1)}\|^2_F \leq - \frac{1}{2},\) we have
\[
L(\hat{Y}_{(k,\ell)}) \leq L(\hat{Y}_{(k,\ell-1)}) - \frac{\eta^{k(k,\ell-1)}_\ell}{2} \|J^{(k,\ell-1)}\|^2_F.
\]

By summing up the above, we have
\[
\sum_{s=0}^{k-1} \sum_{\ell=1}^L \frac{\eta^{(k,s,\ell-1)}_\ell}{2} \|J^{(k,s,\ell-1)}\|^2_F \leq \sum_{s=0}^{k-1} \sum_{\ell=1}^L \left( L(\hat{Y}_{(s,\ell-1)}) - L(\hat{Y}_{(s,\ell)}) \right) \leq L(\hat{Y}_{(0,0)}) < \infty.
\]

Therefore, \(\lim_{k \to \infty} \eta^{(k,\ell)}_\ell \|J^{(k,\ell)}\|^2_F = 0\) for any \(0 \leq \ell < L.\) Also, it follows from the above that
\[
\frac{1}{k} \sum_{s=0}^{k-1} \eta^{(k,s,\ell)}_\ell \|J^{(k,s,\ell)}\|^2_F \leq \frac{1}{k} \sum_{s=0}^{k-1} \sum_{\ell=1}^L \eta^{(k,s,\ell)}_\ell \|J^{(k,s,\ell)}\|^2_F \leq \frac{2}{k} L(\hat{Y}_{(0,0)}) = O\left(\frac{1}{k}\right).
\]

Furthermore, for all \(0 \leq \ell < L,\) if \(0 < \inf_k \eta^{(k,\ell)}_\ell \leq \sup_k \eta^{(k,\ell)}_\ell \leq 1,\) we conclude that \(\lim_{k \to \infty} \|J^{(k,\ell)}\|^2_F = 0\) and \(\lim_{k \to \infty} \eta^{(k,\ell)}_\ell J^{(k,\ell)} = 0.\) For each \(\ell,\) \(\lim_{k \to \infty} W^{(k)}_\ell = W^{(k)}_\ell.\) That is, the BCGD finds a critical point. Since all local minima are global (see, Laurent and Brecht (2018)), \(\{W^{(k)}_\ell\}_{\ell=1}^L\) is a global minimizer.

\[
\text{\hfill \blacksquare}
\]
Appendix F. Proof of Theorem 8

**Proof**  For notational convenience, for $j > i$, let

$$W_{j:i} := W_j W_{j-1} \cdots W_i.$$  

By definition, it follows from the update rule that

$$W^{\ell_k (\ell_{k+1})}_{\ell_k} = W^{\ell_k (\ell_{k+1})}_{\ell_k} - \eta_{\ell_k} (W^{\ell_k}_{\ell_{k+1}:1} X_{:i} : j, \ell_k, W^{\ell_k}_{\ell_{k+1}:1})^T,$$

where $\ell_k$ is randomly chosen indices from $[m]$ and and $\ell_k$ is an index from $[L]$. By multiplying $W^{\ell_k}_{\ell_{k+1}:1} X$ from right, $W^{\ell_k}_{\ell_{k+1}:1}$ from left and subtracting $W^* X$ in the both sides, we obtain

$$(W^{\ell_k+1} - W^*) X = (W^{\ell_k} - W^*) X - \eta_{\ell_k} A^{\ell_k} (X_{:i} : j, \ell_k) : (W^{\ell_k}_{\ell_{k+1}:1} X_{:i} : j) B^{\ell_k} X$$

where

$$A^{\ell_k} := W^{\ell_k}_{\ell_{k+1}:1} (W^{\ell_k}_{\ell_{k+1}:1})^T \in \mathbb{R}^{d_{out} \times d_{out}}, \quad B^{\ell_k} := (W^{\ell_k}_{\ell_{k+1}:1})^T W^{\ell_k}_{\ell_{k+1}:1} \in \mathbb{R}^{d_{in} \times d_{in}}.$$  \hspace{1cm} (41)

Since $A^{\ell_k}$ is symmetric, they are diagonalizable. Thus,

$$(U^{\ell_k} X_{\ell_k})^T A^{\ell_k} U^{\ell_k} = D^{\ell_k} = \text{diag}(\lambda^{\ell_k}), \quad 1 \leq i \leq d_{out},$$

where $U^{\ell_k}$ is orthogonal. Let $\Delta^{\ell_k}_W := W^{\ell_k} - W^*$ and $\Delta^{\ell_k} := \Delta^{\ell_k}_W X$. Since $\ell(a; b) = (a - b)^2/2$, we have

$$\Delta^{\ell_k+1} = \Delta^{\ell_k} - \eta_{\ell_k} A^{\ell_k} \left( \Delta^{\ell_k}_W (X_{:i} : j) X_{:i}^T - (y^{\ell_k} - W^* x^{\ell_k}) (X_{:i} : j)^T \right) B^{\ell_k} X.$$

Let $E = Y - W^* X$ and $E_{:i} := y^{\ell_k} - W^* x^{\ell_k}$. Then

$$(U^{\ell_k})^T \Delta^{\ell_k+1} = (U^{\ell_k})^T \Delta^{\ell_k} - \eta_{\ell_k} D^{\ell_k} (U^{\ell_k})^T \left( \Delta^{\ell_k}_W (X_{:i} : j) X_{:i}^T - E_{:i} (X_{:i} : j)^T \right) B^{\ell_k} X.$$  \hspace{1cm} (42)

Let $\tilde{\Delta}^{\ell_k}_{E, i, \ell} = (U^{\ell_k})^T \Delta^{\ell_k}$. Then

$$\tilde{\Delta}^{\ell_k}_{E, i, \ell} = \eta_{\ell_k} D^{\ell_k} (U^{\ell_k})^T \left( \Delta^{\ell_k}_W (X_{:i} : j) X_{:i}^T - E_{:i} (X_{:i} : j)^T \right) B^{\ell_k} X.$$  \hspace{1cm} (42)

Let $u^{\ell_k}_{l, j}$ be the $j$-th column of $U^{\ell_k}_{l, j}$. The $j$-th row of (42) satisfies

$$\| (\tilde{\Delta}^{\ell_k+1}_{E, i, \ell})_{:j} \|^2 = \| (u^{\ell_k}_{l, j})^T \Delta^{\ell_k} - \eta_{\ell_k} \lambda^{\ell_k} (u^{\ell_k}_{l, j})^T \left( \Delta^{\ell_k}_W (X_{:i} : j) X_{:i}^T - E_{:i} (X_{:i} : j)^T \right) B^{\ell_k} X \|^2$$

$$= \| (\tilde{\Delta}^{\ell_k}_{E, i, \ell})_{:j} \|^2 + \left( \eta_{\ell_k} \lambda^{\ell_k} \right)^2 \| (u^{\ell_k}_{l, j})^T (\Delta^{\ell_k}_W (X_{:i} : j) - E_{:i} (X_{:i} : j)^T) B^{\ell_k} X \|^2$$

$$- 2 \eta_{\ell_k} \lambda^{\ell_k} (u^{\ell_k}_{l, j})^T (\Delta^{\ell_k}_W (X_{:i} : j) - E_{:i} (X_{:i} : j)^T) B^{\ell_k} X \| (\Delta^{\ell_k}_W (X_{:i} : j) - E_{:i} (X_{:i} : j)^T) T u^{\ell_k}_{l, j}.$$  \hspace{1cm} (42)

Note that

$$\| (u^{\ell_k}_{l, j})^T (\Delta^{\ell_k}_W (X_{:i} : j) - E_{:i} (X_{:i} : j)^T) B^{\ell_k} X \|^2$$

$$= \| X_{:i} : j B^{\ell_k} X \|^2 (\| (u^{\ell_k}_{l, j})^T \Delta^{\ell_k}_W (X_{:i} : j) \|^2 + \| (u^{\ell_k}_{l, j})^T E_{:i} (X_{:i} : j) \|^2 - 2 (u^{\ell_k}_{l, j})^T \Delta^{\ell_k}_W (X_{:i} : j) E_{:i} (X_{:i} : j)^T u^{\ell_k}_{l, j}).$$
Thus,

\[
\|(\tilde{\Delta}^{k+1})_j\|^2 = \|(\Delta^k)_j\|^2 - 2\eta_{\ell_k}^k \lambda_{\ell_k,j}^k (u_{\ell_k,j}^k)^T \Delta W^k (X_{i\kappa} X_{i\kappa}^T) \tilde{B}_{\ell_k}^k X (\Delta^k)^T u_{\ell_k,j}^k
\]

\[
+ \left(\frac{\eta_{\ell_k}^k \lambda_{\ell_k,j}^k}{\eta_{\ell_k}^k \lambda_{\ell_k,j}^k}\right)^2 \left(\frac{\|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|}{\|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|^2}\right) \|\Delta W^k X_{i\kappa}\|^2 + \|u_{\ell_k,j}^k\|_2^2
\]

\[
- 2(u_{\ell_k,j}^k)^T \Delta W^k X_{i\kappa} (\mathcal{E}_{;i\kappa})^T u_{\ell_k,j}^k) + 2\eta_{\ell_k}^k \lambda_{\ell_k,j}^k (u_{\ell_k,j}^k)^T \Delta W^k \tilde{B}_{\ell_k}^k X X_{i\kappa} (\mathcal{E}_{;i\kappa})^T u_{\ell_k,j}^k.
\]

Let

\[
B_{\ell_k}^k = X^T (W_{\ell_k}^{k-1})^T W_{\ell_k}^k (\ell_k - 1)! X.
\]

Let us reparameterize the learning rate as \(\eta_{\ell_k}^k = \eta_{\ell_k}^k / \|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|^2\) and define a discrete probability distribution \(\pi\) on \([m]\) to be \(\pi(i) = \|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|^2 / \|X^T \tilde{B}_{\ell_k}^k X\|^2\) for \(1 \leq i \leq m\). Since

\[
X_{i\kappa}^T = X (Y (I - X^T X)^T) = X (I - X^T X) Y^T = (X - XX^T X)^T Y^T = 0,
\]

we have \(E_{i\kappa} \left[ \frac{X_{i\kappa} (\mathcal{E}_{;i\kappa})^T}{\|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|^2} \right] = \frac{X_{i\kappa}^T}{\|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|^2} = 0\). By taking the expectation \(E_{i\kappa}\) with respect to \(i_k \sim \pi\), we obtain

\[
E_{i\kappa} \left[ \|(\tilde{\Delta}^{k+1})_j\|_2^2 \right] = \|(\Delta^k)_j\|^2 - 2\eta_{\ell_k}^k \lambda_{\ell_k,j}^k (u_{\ell_k,j}^k)^T \Delta W^k E_{i\kappa} \left[ \frac{X_{i\kappa} X_{i\kappa}^T}{\|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|^2} \right] \tilde{B}_{\ell_k}^k X (\Delta^k)^T u_{\ell_k,j}^k
\]

\[
+ \left(\frac{\eta_{\ell_k}^k \lambda_{\ell_k,j}^k}{\eta_{\ell_k}^k \lambda_{\ell_k,j}^k}\right)^2 \left(\frac{\|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|}{\|X_{i\kappa}^T \tilde{B}_{\ell_k}^k X\|^2}\right) \|\Delta W^k X_{i\kappa}\|^2 + \|u_{\ell_k,j}^k\|_2^2
\]

\[
- 2(u_{\ell_k,j}^k)^T \Delta W^k X_{i\kappa} (\mathcal{E}_{;i\kappa})^T u_{\ell_k,j}^k) + 2\eta_{\ell_k}^k \lambda_{\ell_k,j}^k (u_{\ell_k,j}^k)^T \Delta W^k \tilde{B}_{\ell_k}^k X X_{i\kappa} (\mathcal{E}_{;i\kappa})^T u_{\ell_k,j}^k.
\]

Suppose

\[
0 < \eta_{\ell_k}^k < \frac{2\lambda_{\min}(B_{\ell_k}^k)}{\lambda_{\max}(A_{\ell_k}^k)}
\]

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and let $M_{\ell,k}^{j} := -\tilde{\eta}_{\ell,k}^{j} k_{k}^{j} I + 2B_{\ell,k}^{j}$. Then, since $\lambda_{\text{min}}(M_{\ell,k}^{j}) = 2\lambda_{\text{min}}(B_{\ell,k}^{j}) - \eta_{\ell,k}^{j} \gamma_{k}^{j} > 0$, $M_{\ell,k}^{j}$ is a positive definite symmetric matrix for all $j$. Thus,

$$
E_{k}[[\Delta_{k+1}^{j}]^{2}] 
\leq \|\Delta_{k}^{j}\|^{2} - \frac{\eta_{\ell,k}^{j} \lambda_{\text{min}}(M_{\ell,k}^{j})}{\|W_{(\ell-1):1}^{k}\|^{4}_{F}} \|\Delta_{k}^{j}\|^{2} + \frac{\eta_{\ell,k}^{j} \lambda_{\text{max}}(M_{\ell,k}^{j})}{\|W_{(\ell-1):1}^{k}\|^{4}_{F}} \|\Delta_{k}^{j}\|^{2}.
$$

and similarly, we have

$$
E_{k}[[\Delta_{k+1}^{j}]^{2}] 
\geq \left(1 - \frac{\eta_{\ell,k}^{j} \lambda_{\text{min}}(M_{\ell,k}^{j})}{\|W_{(\ell-1):1}^{k}\|^{4}_{F}} \right) \|\Delta_{k}^{j}\|^{2} + \frac{\eta_{\ell,k}^{j} \lambda_{\text{max}}(M_{\ell,k}^{j})}{\|W_{(\ell-1):1}^{k}\|^{4}_{F}} \|\Delta_{k}^{j}\|^{2}.
$$

Since

$$
-\tilde{\eta}_{\ell,k}^{j} k_{k}^{j} \lambda_{\text{min}}(M_{\ell,k}^{j}) = -\tilde{\eta}_{\ell,k}^{j} \gamma_{\ell,k,i}^{j} (2\lambda_{\text{min}}(B_{\ell,k}^{j}) - \eta_{\ell,k}^{j} \gamma_{k}^{j}) = \left((\tilde{\eta}_{\ell,k}^{j} \gamma_{\ell,k,i}^{j}) - \lambda_{\text{min}}(B_{\ell,k}^{j})\right)^{2} - \lambda_{\text{min}}^{2}(B_{\ell,k}^{j})
$$

if we set $\tilde{\eta}_{\ell,k}^{j} = \eta_{\ell,k}^{j} \lambda_{\text{min}}(A_{\ell,k}^{j})$, where $0 < \eta < 2$, we have

$$
-\tilde{\eta}_{\ell,k}^{j} k_{k}^{j} \lambda_{\text{min}}(M_{\ell,k}^{j}) \leq -\lambda_{\text{min}}^{2}(B_{\ell,k}^{j}) \left(1 - (1 - \eta/\kappa(A_{\ell,k}^{j}))^{2}\right) = -\gamma_{k}^{j}.
$$

Thus, we obtain

$$
E_{k}[[\Delta_{k+1}^{j}]^{2}] \leq \left(1 - \frac{\gamma_{k}^{j}}{\|W_{(\ell-1):1}^{k}\|^{4}_{F}} \right) \|\Delta_{k}^{j}\|^{2} + \frac{\eta^{2} \lambda_{\text{min}}^{2}(B_{\ell,k}^{j})}{\|W_{(\ell-1):1}^{k}\|^{4}_{F}} \|\Delta_{k}^{j}\|^{2}.
$$

By summing up with respect to $j$, we have

$$
E_{k}[[\Delta_{k+1}^{j}]^{2}] \leq \left(1 - \frac{\left(1 - (1 - \eta/\kappa(W_{L(\ell+1)}^{k}))^{2}\right)}{\tilde{\kappa}^{4}(\|W_{(\ell-1):1}^{k}\|^{4}_{F})} \right) \|\Delta_{k}^{j}\|^{2} + \frac{\eta^{2} \|\Delta_{k}^{j}\|^{2}}{\tilde{\kappa}^{4}(\|W_{(\ell-1):1}^{k}\|^{4}_{F})},
$$

where $\tilde{\kappa}(\cdot)$ is the scaled condition number defined to be

$$
\tilde{\kappa}(X) = \frac{\|X\|_{F}}{\sigma_{\text{min}}(X)}.
$$
Similarly, since
\[ \eta_{k}^{k_{k}} \lambda_{k_{k}}^{k_{k}} \lambda_{k_{k}}^{k_{k}} (M_{k_{k}}^{k_{k}}) = 2 \lambda_{\max}(B_{k_{k}}^{k_{k}}) (\eta_{k_{k}}^{k_{k}} \lambda_{k_{k}}^{k_{k}}) - (\eta_{k_{k}}^{k_{k}} \lambda_{k_{k}}^{k_{k}})^{2} \]
\[ = \lambda_{\max}(B_{k_{k}}^{k_{k}}) - \left( (\eta_{k_{k}}^{k_{k}} \lambda_{k_{k}}^{k_{k}}) - \lambda_{\max}(B_{k_{k}}^{k_{k}}) \right)^{2} \]
\[ = \lambda_{\max}(B_{k_{k}}^{k_{k}}) - \left( \eta_{\lambda_{k_{k}}^{k_{k}}}^{k_{k}} \lambda_{\lambda_{k_{k}}}^{k_{k}} \lambda_{\lambda_{k_{k}}}^{k_{k}} - \lambda_{\max}(B_{k_{k}}^{k_{k}}) \right)^{2} \]
\[ \leq \lambda_{\max}(B_{k_{k}}^{k_{k}}) \left( 1 - \left( 1 - \frac{\eta}{\kappa(B_{k_{k}}^{k_{k}})} \right)^{2} \right), \]
we have
\[
E_{k_{k}} \left[ ||\Delta_{k_{k}+1}^{k_{k}}||_{F}^{2} \right] \geq \left( 1 - \frac{\lambda_{\max}(B_{k_{k}}^{k_{k}}) \left( 1 - \left( 1 - \frac{\eta}{\kappa(B_{k_{k}}^{k_{k}})} \right)^{2} \right)}{||W_{k_{k}}^{k_{k}}(k_{k}-1):1X||_{F}^{4}} \right) \|\tilde{\Delta}_{k_{k}}^{k_{k}}\|_{F}^{2} + \frac{\eta^{2}||E||_{F}^{2}}{\kappa^{4}(W_{k_{k}}^{k_{k}}(k_{k}+1):k_{k}^{4}(W_{k_{k}}^{k_{k}}(k_{k}-1):1X))}. \]

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