Notation. We use \( \| \cdot \| \) to represent the Euclidean norm of a vector and Frobenius norm of a matrix.
We use \( \nabla \) to denote the Jacobian of a vector-valued and gradient of a scalar-valued function and
\( \nabla \Phi(a) \{ b \} \) to represent the directional derivative of \( \Phi \) along \( b \). We use \( \odot \) and \( \otimes \) to denote the
Hadamard (entry-wise) product and Kronecker product, respectively. For \( A \in \mathbb{R}^{m \times n} \) and \( t \in \mathbb{Z}_+ \), we
denote \( A^{t} \in \mathbb{R}^{m \times n} \) with its \( t \)-th column defined as \( \text{vec}(x_n \odot \cdots \odot x_1) \in \mathbb{R}^{m^t} \). We use lower-case
bold font to denote vectors. Sets and scalars are represented by calligraphic and standard fonts,
respectively. We use \([n]\) to denote \( \{1, \cdots, n\} \) for an integer \( n \). We use \( O \) and \( \Omega \) to hide logarithmic
factors and use \( \lesssim \) to ignore terms up to constant and logarithmic factors.

A Proof of Lemma 1

Intuitively, if \( \nabla \Phi^*(w_0) \) is a \( (\mu_\Phi, \nu_\Phi) \)-near-isometry, then one would expect \( \nabla \Phi^* \) to remain near-isometry for all nearby points. Formally, let \( A, B \in \mathbb{R}^{m \times n} \) and let singular values of a matrix are
ordered such that \( \sigma_i(A) \geq \sigma_j(A) \) and \( \sigma_i(B) \geq \sigma_j(B) \) for \( 1 \leq i \leq j \leq \min\{m, n\} \). Using Weyl’s
inequality and for \( i + j - 1 \leq \min\{m, n\} \), we have:

\[
\sigma_{i+j-1}(A + B) \leq \sigma_i(A) + \sigma_j(B). \tag{A.1}
\]

More formally, suppose that \( w \in \mathbb{R}^d \) satisfies

\[
\|w - w_0\| \leq \frac{\mu_\Phi}{2 \beta_\Phi} = \rho_\Phi. \tag{A.2}
\]

If \( \nabla \Phi^*(w_0) \) is \( (\mu_\Phi, \nu_\Phi) \)-isometry in the sense of Definition 1, then applying Weyl’s inequality \( (A.1) \)
along with using smoothness and \( (A.2) \), we have

\[
\sigma_{\min}(\nabla \Phi^*(w)) \geq \sigma_{\min}(\nabla \Phi^*(w_0)) - \sigma_{\max}(\nabla \Phi^*(w) - \nabla \Phi^*(w_0))
\geq \frac{\mu_\Phi - \beta_\Phi \|w - w_0\|}{2}.
\]

Using a similar argument, we establish an upper bound \( \sigma_{\max}(\nabla \Phi^*(w)) \):

\[
\sigma_{\max}(\nabla \Phi^*(w)) \leq \sigma_{\max}(\nabla \Phi^*(w_0)) + \sigma_{\max}(\nabla \Phi^*(w) - \nabla \Phi^*(w_0)) \leq \nu_\Phi + \frac{\mu_\Phi}{2} \leq \frac{3\nu_\Phi}{2}.
\]

B Proof of Lemma 2

Let \( t \geq 0 \) and denote

\[
\z(t) = \Phi(\gamma(t)) \tag{A.3}
\]

so we have

\[
h(\gamma(t)) = f(\Phi(\gamma(t)) = f(\z(t)). \tag{A.4}
\]

Taking the first-order derivative w.r.t. \( t \), we have

\[
\dot{\z}(t) = \nabla \Phi(\gamma(t)) \{ \dot{\gamma}(t) \}
= -\nabla h(\gamma(t)) \{ \nabla h(\gamma(t)) \}. \tag{A.5}
\]

Note that we have

\[
\frac{dh(\gamma(t))}{dt} = \nabla h(\gamma(t)) \{ \dot{\gamma}(t) 
= -\nabla h(\gamma(t)) \{ \nabla h(\gamma(t)) \}
= -\|\nabla h(\gamma(t))\|^2. \tag{A.6}
\]
Length of the segment of the curve $\gamma_K$ restricted to the interval $[0,t]$ is given by
\[
\ell(t) = \int_0^t \|\dot{\gamma}(\tau)\| \, d\tau \\
= \int_0^t \|\nabla h(\gamma(\tau))\| \, d\tau \\
\leq \int_0^t \sigma_{\text{max}}(\nabla \Phi^*(\gamma(\tau)) \cdot \|\nabla f(\zeta(\tau))\| \, d\tau \\
\lesssim \nu \Phi \int_0^t \|\nabla f(\zeta(\tau))\| \, d\tau.
\] (A.7)

To control the norm in the last line of (A.7), we note that
\[
-\frac{d}{dt} \sqrt{f(\zeta(\tau)) - f(\zeta(t))} = - \frac{df(\zeta(\tau))}{d\tau} \\
= - \frac{\langle \nabla f(\zeta(\tau)), \dot{\zeta}(\tau) \rangle}{2\sqrt{f(\zeta(\tau)) - f(\zeta(t))}} \\
= \frac{\langle \nabla f(\zeta(\tau)), \nabla \Phi(\gamma(\tau)) \cdot \nabla h(\gamma(\tau)) \rangle}{2\sqrt{f(\zeta(\tau)) - f(\zeta(t))}} \\
\geq \frac{\sigma_{\text{min}} f(\gamma(\tau)) \cdot \|\nabla f(\zeta(\tau))\|}{2\sqrt{f(\zeta(\tau)) - f(\zeta(t))}} \\
\geq \frac{\sigma_{\text{min}}^2 f(\gamma(\tau)) \cdot \|\nabla f(\zeta(\tau))\|^2}{2\sqrt{f(\zeta(\tau)) - f(\zeta(t))}} \\
\geq \frac{\alpha_T \mu_\Phi^2 \cdot \|\nabla f(\zeta(\tau))\|^2}{\|\nabla f(\zeta(\tau))\|} \\
= \sqrt{\alpha_T \mu_\Phi^2} \cdot \|\nabla f(\zeta(\tau))\|
\] (A.8)
provided that the denominators are nonzero. Substituting (A.8) into (A.7), the desired length is bounded by
\[
\ell(t) \lesssim \nu \Phi \int_0^t \|\nabla f(\zeta(\tau))\| \, d\tau \\
\lesssim \frac{\nu \Phi}{\mu_\Phi^2 \sqrt{\alpha_T}} \int_0^t \frac{d}{dt} \sqrt{f(\zeta(\tau)) - f(\zeta(t))} \, d\tau \\
= \frac{\nu \Phi}{\mu_\Phi^2 \sqrt{\alpha_T}} \left( \sqrt{f(\zeta(0)) - f(\zeta(t))} \right) \\
\leq \frac{\nu \Phi \sqrt{f(\zeta(0))}}{\mu_\Phi^2 \sqrt{\alpha_T}} \\
= \frac{\nu \Phi \sqrt{h(\gamma(0))}}{\mu_\Phi^2 \sqrt{\alpha_T}} \\
= \frac{\nu \Phi \sqrt{h(w_0)}}{\mu_\Phi^2 \sqrt{\alpha_T}},
\]
which completes the proof of Lemma 2.

\section{Proof of Theorem 2}

The proof is along the lines of Theorem 1. We first compute the length of the trajectory traversed by gradient descent iterates. Formally, let $I$ denote the first iteration such that $w_I \not\in \text{ball}(w_0, \rho_\Phi)$. The
where the fourth inequality holds since
\[ \| f(z) - f(z_i) \| \geq \langle z_i - z_i+1, \nabla f(z_i) \rangle - \frac{\beta_f}{2} \| z_i+1 - z_i \|^2. \]

This following lemma is useful for our proof.

**Lemma A.1.** Suppose \( u, v \in \text{ball}(w_0, \rho_u) \). Then we have
\[ \| \Phi(u) - \Phi(v) \| \leq \frac{3\rho_u}{2} \| u - v \|. \]

**Proof.** Using Lemma 1, we establish a bound on \( \| \Phi(u) - \Phi(v) \| \):
\[
\| \Phi(u) - \Phi(v) \| = \left\| \int_0^1 \nabla \Phi(v + t(u - v))(u - v) \, dt \right\|
\leq \int_0^1 \| \nabla \Phi(v + t(u - v))(u - v) \| \, dt
\leq \frac{3\rho_u}{2} \| u - v \|.
\]

Let \( i \leq I - 2 \). To control the upper bound in (A.9), we use the smoothness of \( f \) and Lemma A.1 to obtain a standard “descent inequality” as:
\[
f(z_i) - f(z_i+1) \geq \langle z_i - z_i+1, \nabla f(z_i) \rangle - \frac{\beta_f}{2} \| z_i+1 - z_i \|^2
= \langle \Phi(w_i) - \Phi(w_{i+1}), \nabla f(z_i) \rangle - \frac{\beta_f}{2} \| \Phi(w_{i+1}) - \Phi(w_i) \|^2
\]
\[
\geq \langle \nabla \Phi(w_i) \{ w_i - w_{i+1} \}, \nabla f(z_i) \rangle - \frac{\beta_f}{2} \| \Phi(w_{i+1}) - \Phi(w_i) \|^2
- \frac{\beta_f}{2} \| w_{i+1} - w_i \|^2 \| \nabla f(z_i) \|
\geq \langle \nabla \Phi(w_i) \{ w_i - w_{i+1} \}, \nabla f(z_i) \rangle - \frac{1}{2} \| w_{i+1} - w_i \|^2 \left( \beta_f \| \nabla f(z_i) \| + \frac{9\beta_f \nu^2_\Phi}{4} \right)
\geq \eta \| \nabla h(w_i) \|^2 - \frac{\eta^2}{2} \| \nabla h(w_i) \|^2 \left( \beta_f \| \nabla f(z_i) \| + \frac{9\beta_f \nu^2_\Phi}{4} \right)
= \eta \| \nabla h(w_i) \|^2 \left( 1 - \frac{\eta \beta_f \| \nabla f(z_i) \|^2}{2} - \frac{9\eta \beta_f \nu^2_\Phi}{8} \right)
\geq \eta \nu^2_\Phi \| \nabla f(z_i) \|^2 \text{ (chain rule and Lemma 1)}
\]
where the fourth inequality holds since
\[ \| \Phi(a) - \Phi(b) - \nabla \Phi(b)(a - b) \| \leq \frac{\beta_f}{2} \| b - a \|^2 \]
for \( \beta_f \)-smooth \( \Phi \), and the last line holds provided that \( \eta \) satisfies:
\[
\eta \lesssim \frac{1}{\beta_f \max_i \| \nabla f(z_i) \| + \beta_f \nu^2_\Phi}.
\]
We now use the bound above to find an upper bound on $\sqrt{f(z_i) - f(z_{i-1})} - \sqrt{f(z_{i+1}) - f(z_{i-1})}$:

$$\sqrt{f(z_i) - f(z_{i-1})} - \sqrt{f(z_{i+1}) - f(z_{i-1})} = \frac{f(z_i) - f(z_{i+1})}{\sqrt{f(z_i) - f(z_{i-1})} + \sqrt{f(z_{i+1}) - f(z_{i-1})}} \geq \frac{\eta \mu^2}{2} \|\nabla f(z_i)\|$$

Substituting (A.11) into (A.9), we have

$$\ell(I) \lesssim \eta \mu \Phi \sum_{i=0}^{l-1} \|\nabla f(z_i)\|$$

$$\lesssim \frac{\nu \Phi \sqrt{\alpha f \mu^2}}{\alpha f \mu^2} \sum_{i=0}^{l-2} \left( \sqrt{\nabla f(z_i) - f(z_{i-1})} - \sqrt{f(z_{i+1}) - f(z_{i-1})} \right) + \eta \mu \Phi \|\nabla f(z_{l-1})\|$$

$$\lesssim \frac{\nu \Phi \sqrt{f(z_0) - f(z_{l-1})} + \eta \mu \Phi \|\nabla f(z_{l-1})\|}{\sqrt{\alpha f \mu^2}}$$

Note that

$$f(z_0) = h(w_0) \lesssim \frac{\alpha f \mu^2}{\beta^2 \nu^2}$$

and scaling down the learning rate sufficiently to control the second term in the upper bound ensure that

$$\ell(I) \leq \frac{\rho \Phi}{2} = \frac{\mu \Phi}{4 \beta \Phi}$$

Hence, the gradient descent iterates satisfy:

$$\{w_i\}_{i \geq 0} \in \text{ball}(w_0, \rho \Phi),$$

which implies that the limit $\Phi$ exists and is globally optimal. In the following, we simplify the expression for $\eta$ in (A.10). Since the iterates of gradient flow remain within a ball of radius $\rho \Phi$, we can compute the local Lipschitz constant of $f$ as

$$\max_i \|\nabla f(z_i)\| \leq \|\nabla f(z_0)\| + \max_i \|\nabla f(z_i) - \nabla f(z_0)\|$$

$$\leq \|\nabla f(z_0)\| + \beta f \max_i \|z_i - z_0\|$$

$$= \|\nabla f(z_0)\| + \beta f \max_i \|\Phi(w_i) - \Phi(w_0)\|$$

$$\leq \|\nabla f(z_0)\| + \frac{3 \beta f \nu^2 \Phi}{2} \max_i \|w_i - w_0\|$$

$$\leq \|\nabla f(z_0)\| + \frac{3 \beta f \nu^2 \Phi}{2} \cdot \rho \Phi$$

$$= \|\nabla f(z_0)\| + \frac{3 \beta f \mu^2 \nu^2 \Phi}{4 \beta \Phi}.$$
Substituting (A.13) into (A.10), an upper bound on \( \eta \) is given by
\[
\eta \leq \frac{1}{\beta_\phi \| \nabla f(z_0) \| + \beta_f \mu_\phi \nu_\phi + \beta_f \nu_\phi^2} \leq \frac{1}{\beta_\phi \| \nabla f(z_0) \| + \beta_f \mu_\phi^2 + \beta_f \nu_\phi^2}
\] (A.14)
where the last inequality holds since \( \mu_\phi \leq \nu_\phi \).

Finally, using (7), we prove the linear convergence to the limit point \( w \):
\[
h(w_{i+1}) = h(w_{i+1}) - h(w_i) + h(w_i)
\]
\[
= f(z_{i+1}) - f(z_i) + h(w_i)
\]
\[
\leq -C \mu_\phi^2 \| \nabla f(z_i) \|^2 + h(w_i)
\]
\[
\leq (1 - C \eta \bar{\alpha}_f \mu_\phi^2) h(w_i)
\] (A.15)
where \( C \) is a universal constant. This completes the proof of Theorem 2.

D Proof of Lemma 3

We first obtain the expression for adjoint operator \( \nabla \Phi^*(\Theta) : \mathbb{R}^{d_2 \times n} \to \mathbb{R}^{d_1 \times d_0} \times \mathbb{R}^{d_2 \times d_1} \). Let \( \Delta_W \in \mathbb{R}^{d_1 \times d_0} \), \( \Delta_V \in \mathbb{R}^{d_2 \times d_1} \), and \( \Delta \in \mathbb{R}^{d_2 \times n} \). We expand \( \Phi \) as follow:
\[
\Phi(W + \Delta_W, V) \approx \Phi(W, V) + \nabla_W \Phi(\Delta_W),
\]
\[
\Phi(W, V + \Delta_V) \approx \Phi(W, V) + \nabla_V \Phi(\Delta_V)
\] (A.16)
where
\[
\nabla_W \Phi(\Delta_W) = V \left( \hat{\phi}(W \Delta) \right), \quad \nabla_V \Phi(\Delta_V) = \Delta \phi(WX)
\]
\( \odot \) stands for the Hadamard (entry-wise) product, and \( \hat{\phi}(W \Delta) \) is the derivative of \( \phi \) calculated at each entry of the matrix \( W \Delta \). The operator \( \nabla \Phi(\Theta) \) is given by \( \langle \Delta_W, \Delta_V \rangle \to \nabla_W \Phi(\Delta_W) + \nabla_V \Phi(\Delta_V) \).

Using the cyclic property of the trace operator and trace \( (A \odot B)C = \text{trace} ((A \odot C^\top)B^\top) \), we have
\[
\langle \Delta, \nabla_W \Phi(\Delta_W) \rangle = \left\langle \left( \hat{\phi}(W \Delta) \odot V^\top \Delta \right) X^\top, \Delta_W \right\rangle,
\]
\[
\langle \Delta, \nabla_V \Phi(\Delta_V) \rangle = \left\langle \Delta_V, \Delta \phi(X^\top W^\top) \right\rangle.
\] (A.17)

Substituting (A.17), the adjoint operator is given by
\[
\nabla \Phi^*(\Theta) : \Delta \to \left( \left( \hat{\phi}(W \Delta) \odot V^\top \Delta \right) X^\top, \Delta \phi(X^\top W^\top) \right).
\] (A.18)

Suppose that there exist \( \hat{\phi}_{\max}, \hat{\phi}_{\max} < \infty \) such that
\[
\sup_a |\hat{\phi}(a)| \leq \hat{\phi}_{\max}, \quad \sup_a |\hat{\phi}(a)| \leq \hat{\phi}_{\max}.
\] (A.19)

Lemma A.2. Let \( A \in \mathbb{R}^{m \times n} \) and \( B \in \mathbb{R}^{n \times k} \). Then, we have
\[
\sigma_{\min}(A) \| B \| \leq \| AB \| \leq \sigma_{\max}(A) \| B \|.
\]

Using Lemma A.2 and triangular inequality, we note that
\[
\| \nabla \Phi^*(\Theta, \Delta) \| \leq \left\| \left( \hat{\phi}(W \Delta) \odot (V^\top \Delta) \right) X^\top \right\| + \| \Delta \phi(X^\top W^\top) \|
\]
\[
\leq \hat{\phi}_{\max} \sigma_{\max}(X) \sigma_{\max}(V) \| \Delta \| + \sigma_{\max}(\phi(WX)) \| \Delta \|.
\] (A.20)

Similarly, we have this lower bound:
\[
\| \nabla \Phi^*(\Theta, \Delta) \| \geq \sigma_{\min}(\phi(WX)) \| \Delta \|.
\] (A.21)
Substituting $\Theta_0 = (W_0, V_0)$ into (A.20) and (A.21), $\mu_\Phi$ and $\nu_\Phi$ are given by:

\[
\begin{align*}
\sigma_{\max}(\nabla \Phi^* (\Theta_0)) &\leq \tilde{\phi}_{\max} \sigma_{\max}(X) \sigma_{\max}(V_0) + \sigma_{\max}(\phi(W_0 X)) =: \nu_\Phi, \\
\sigma_{\min}(\nabla \Phi^* (\Theta_0)) &\geq \sigma_{\min}(\phi(W_0 X)) =: \mu_\Phi.
\end{align*}
\] (A.22)

In the following, we find the smoothness parameter $\beta_\Phi$ in (4). Let $\Theta, \hat{\Theta} \in \mathbb{R}^{d_1 \times d_0} \times \mathbb{R}^{d_2 \times d_1}$. We note that $\|\nabla \Phi(\Theta, \Delta) - \nabla \Phi(\hat{\Theta}, \Delta)\| \leq U_1 + U_2$ where

\[
\begin{align*}
U_1 &= \|V(\phi(W^T X) \circ (\Delta W^T X)) - \hat{V}(\hat{\phi}(W^T X) \circ (\Delta W^T X))\| \\
U_2 &= \|\Delta V \phi(W^T X) - \Delta V \hat{\phi}(W^T X)\|.
\end{align*}
\] (A.23)

Let us denote

\[
\sigma_{\max}(\hat{V}) \leq \chi_{\max}.
\] (A.24)

An upper bound on $U_1$ in (A.23) is given by:

\[
\begin{align*}
U_1 &\leq \|(V - \hat{V})(\phi(W^T X) \circ (\Delta W^T X))\| + \|\hat{V}(\hat{\phi}(W^T X) \circ (\Delta W^T X) - \hat{V}) \phi(W^T X) \circ (\Delta W^T X))\| \\
&\leq \tilde{\phi}_{\max} \sigma_{\max}(X) \|V - \hat{V}\| \|\Delta W\| + \sigma_{\max}(X) \sigma_{\max}(\tilde{V}) \|\phi(W^T X) - \hat{\phi}(W^T X)\| \|\Delta W\| \\
&\leq \tilde{\phi}_{\max} \sigma_{\max}(X) \|V - \hat{V}\| \|\Delta W\| + \sigma_{\max}(X) \|\Delta W\| \|\Delta W\|. \\
\end{align*}
\]

An upper bound on $U_2$ in (A.23) is given by:

\[
U_2 \leq \tilde{\phi}_{\max} \sigma_{\max}(X) \|W - \hat{W}\| \|\Delta V\|.
\]

Substituting the upper bounds on $U_1$ and $U_2$, an upper bound on $\sigma_{\max}(\nabla \Phi(\Theta) - \nabla \Phi(\hat{\Theta}))$ is given by

\[
\begin{align*}
\sigma_{\max}(\nabla \Phi(\Theta) - \nabla \Phi(\hat{\Theta})) &\leq \sigma_{\max}(X) \left(\tilde{\phi}_{\max} + \tilde{\phi}_{\max} \chi_{\max}\right) \|W - \hat{W}\| + \sigma_{\max}(X) \|V - \tilde{V}\| \\
&\leq \sqrt{2} \sigma_{\max}(X) \left(\tilde{\phi}_{\max} + \tilde{\phi}_{\max} \chi_{\max}\right) \|\Theta - \hat{\Theta}\|
\end{align*}
\]

where the last inequality holds since

\[
\|W - \hat{W}\| + \|V - \tilde{V}\| \leq \sqrt{2} \sqrt{\|W - \hat{W}\|^2 + \|V - \tilde{V}\|^2}.
\]

Finally, $\beta_\Phi$ in (4) is given by

\[
\beta_\Phi = \sqrt{2} \sigma_{\max}(X) \left(\tilde{\phi}_{\max} + \tilde{\phi}_{\max} \chi_{\max}\right).
\] (A.25)

### E Proof of Theorem 3

This is our setup: $\min_{\Theta \in \mathbb{R}^{d_1 \times d_0} \times \mathbb{R}^{d_2 \times d_1}} h(\Theta)$ where

\[
h(\Theta) = \|V \phi(W X) - Y\|^2.
\]

Note that $\alpha_f = \beta_f = 2$.

Suppose that there exists $\chi_{\max} < \infty$ such that, for all $i \geq 0$, we have

\[
\sigma_{\max}(V_i) \leq \chi_{\max}.
\]

The details of $\chi_{\max}$ later will be provided in Section E.6.

In Lemma 3, we have shown that

\[
\begin{align*}
\mu_\Phi &= \sigma_{\min}(\phi(W_0 X)), \\
\nu_\Phi &= \tilde{\phi}_{\max} \sigma_{\max}(X) \sigma_{\max}(V_0) + \sigma_{\max}(\phi(W_0 X)), \\
\beta_\Phi &= \sqrt{2} \sigma_{\max}(X) \left(\tilde{\phi}_{\max} + \tilde{\phi}_{\max} \chi_{\max}\right).
\end{align*}
\]

In order to apply Theorem 2, we now establish high-probability bounds on random quantities $\mu_\Phi, \nu_\Phi, \text{and } h(\Theta_0)$ given the initialization in (17).
We start with the basic definition of Hermite polynomial and its properties. Let
\[ \mu \]
We now estimate the random quantities \( \mu \). We use the properties of Hermite polynomials \([3][\S 18.18.11]\):
\[ \langle q_i, q_j \rangle_H = \{ i! \quad i = j, \quad 0 \quad i \neq j. \] (A.26)

Using the above orthogonal basis to decompose \( \phi(W_0X) \), we have
\[ \phi(W_0X) = \sum_{i=0}^{\infty} \frac{c_i}{i!} \cdot q_i(W_0X) \] (A.27)
where \( c_i = \langle \phi, q_i \rangle_H \) and each matrix \( q_i(W_0X) \in \mathbb{R}^{d_i \times n} \) is formed by applying \( q_i \) entry-wise to the matrix \( W_0X \). Let us denote
\[ M_0 := \phi(X^TW_0^T)\phi(W_0X). \]

Let \( 0 < \tau < 1 \). Suppose there are constants \( r_1, r_2 \) such that \( \tau r_1^*|\phi(a)| \leq |\phi(\tau a)| \leq \tau r_2^*|\phi(a)| \) for all \( a \). In the following, we first obtain \( \mathbb{E}[M_0] = \mathbb{E}[\phi(X^T\tilde{W}_0^T)\phi(W_0X)] \) with \( W_0 \sim \mathcal{N}(0, 1) \) and then obtain a lower bound on \( \sigma_{\min}(\mathbb{E}[M_0]) \) and an upper bound on \( \sigma_{\min}(\mathbb{E}[M_0]) \) by scaling the variance. Applying Hermite decomposition (A.27) and taking expectation, we have
\[ \mathbb{E}[\tilde{M}_0] = \mathbb{E}\left[ \phi(X^T\tilde{W}_0^T)\phi(W_0X) \right] = \sum_{i,j=0}^{\infty} \frac{c_ic_j}{i!j!} \mathbb{E}[q_i(X^T\tilde{W}_0^T)q_j(\tilde{W}_0X)] \] (A.28)
where the expectation is w.r.t. the random matrix \( \tilde{W}_0 \). Let \( x_a \in \mathbb{R}^{d_a} \) denote the \( a \)-th column of the training data \( X \). Each summand in (A.28) is an \( n \times n \) matrix where
\[ \left[ \mathbb{E}[q_i(X^T\tilde{W}_0^T)q_j(\tilde{W}_0X)] \right]_{a,b} = \sum_{c=1}^{d_1} \mathbb{E} \left[ q_i(x_a^T\tilde{W}_{0,c,\rightarrow})q_j(\tilde{W}_{0,c,\rightarrow}x_b) \right], \] (A.29)
where \( \tilde{W}_{0,c,\rightarrow} \) is the \( c \)-th row of \( \tilde{W}_0 \) for \( a, b \in [n] \).

In summand on the RHS of (A.29), we note that there is a linear combination of \( \tilde{W}_0 \)'s elements inside each Hermite polynomial.
We use the properties of Hermite polynomials \([3][\S 18.18.11]\):
\[ \left( a_1^2 + \cdots + a_r^2 \right)^{\frac{r}{2}} \frac{1}{i!} \hat{q}_i \left( \frac{a_1x_1 + \cdots + a_rx_r}{(a_1^2 + \cdots + a_r^2)^{\frac{r}{2}}} \right) = \sum_{s_1+\cdots+s_r=i} \frac{a_1^{s_1} \cdots a_r^{s_r}}{s_1! \cdots s_r!} \hat{q}_{s_1}(x_1) \cdots \hat{q}_{s_r}(x_r) \] (A.30)
where \( \hat{q}_i \)’s form an orthogonal basis, equipped with the inner product \( \langle u, v \rangle_{\hat{H}} = \frac{1}{\sqrt{\pi}} \int u(x)v(x) \exp(-x^2) \, dx \). This basis follows the physicist’s convention of Hermite polynomial.
Since $\tilde{q}_i$ and $q_i$ are rescalings of the other, we can replace $q_i$'s into (A.30). Note that we have $\|x_a\|_2 = 1$ for all $a \in [n]$. Then we have

$$q_i(x_a^\top \tilde{W}_{0,c,-}) = i! \sum_{s_1 + \cdots + s_{d_0} = i} \frac{x_{a,1}^{s_1} \cdots x_{a,d_0}^{s_{d_0}}}{s_1! \cdots s_{d_0}!} q_{s_1}(\tilde{W}_{0,c,1}) \cdots q_{s_{d_0}}(\tilde{W}_{0,c,d_0}) \tag{A.31}$$

where $x_{a,k}$ and $\tilde{W}_{0,c,k}$ are $k$-th entry of $x_a$ and $\tilde{W}_{0,c,-}$ for $k \in [d_0]$. Using the expansion in (A.31), we expand (A.29) as follows:

$$\zeta_{i,j}(a,b) = \frac{j!}{i!} \sum_{s_1 + \cdots + s_{d_0} = i} \sum_{s'_1 + \cdots + s'_{d_0} = j} \frac{(x_{a,1}^{s_1} x_{b,1}^{s'_1} \cdots x_{a,d_0}^{s_{d_0}} x_{b,d_0}^{s'_{d_0}})^{s_{d_0}'}}{s_1! \cdots s'_{d_0}!} \rho_{s,s'}(\tilde{W}_{0,c,-}) = \begin{cases} (1)! \sum_{s_1 + \cdots + s_{d_0} = i} \frac{(x_{a,1}^{s_1} x_{b,1}^{s'_1} \cdots x_{a,d_0}^{s_{d_0}} x_{b,d_0}^{s'_{d_0}})^{s_{d_0}'}}{s_1! \cdots s'_{d_0}!} \rho_{s,s'}(\tilde{W}_{0,c,-}) & i = j, \\ 0 & i \neq j \end{cases} \tag{A.32}$$

where $\zeta_{i,j}(a,b) = \mathbb{E} \left[ q_i(x_a^\top \tilde{W}_{0,c,-}) q_j(\tilde{W}_{0,c,-}^\top x_b) \right], \rho_{s,s'}(\tilde{W}_{0,c,-}) = \mathbb{E} \left[ q_{s_1}(\tilde{W}_{0,c,1}) \cdots q_{s_{d_0}}(\tilde{W}_{0,c,d_0}) \cdot q_{s'_1}(\tilde{W}_{0,c,1}) \cdots q_{s'_{d_0}}(\tilde{W}_{0,c,d_0}) \right], \mathbf{s} = [s_1, \cdots, s_{d_0}], \text{and } \mathbf{s'} = [s'_1, \cdots, s'_{d_0}].$

To simplify the expression in (A.32), we define $X^{s_i} \in \mathbb{R}^{d_0 \times n}$ where the $a$-th column is given by

$$X^{s_i} = \text{vec}(a \otimes \cdots \otimes a_a) \in \mathbb{R}^{d_0},$$

which is also called Khatri-Rao product. For $i = 0$, we use the convention that $X^{s_0} = 11^\top \in \mathbb{R}^{n \times n}$.

We can rewrite (A.32) as follows:

$$\zeta_{i,j}(a,b) = \begin{cases} i! (X^{s_i}_a, X^{s_i}_b) & i = j, \\ 0 & i \neq j. \end{cases} \tag{A.33}$$

Substituting (A.33) back into (A.29), we find that

$$\mathbb{E} \left[ q_i(X^\top \tilde{W}_0^\top) q_j(\tilde{W}_0 X) \right]_{a,b} = \sum_{i=1}^{d_1} \mathbb{E} \left[ q_i(x_a^\top \tilde{W}_{0,c,-}) q_j(\tilde{W}_{0,c,-}^\top x_b) \right] = \begin{cases} d_1 i! (X^{s_i}_a, X^{s_i}_b) & i = j, \\ 0 & i \neq j. \end{cases} \tag{A.34}$$

Substituting (A.34) into (A.28), we have

$$\mathbb{E} \left[ M_0 \right] = d_1 \left( c_0^2 11^\top + c_0^2 X^\top X + \sum_{i=2}^{\infty} \frac{c_i^2}{i!} (X^{s_i})^\top X^{s_i} \right). \tag{A.35}$$

We now establish an upper bound on $\sigma_{\max} \left( \sum_{i=2}^{\infty} \frac{c_i^2}{i!} (X^{s_i})^\top X^{s_i} \right)$:

$$\sigma_{\max} \left( \sum_{i=2}^{\infty} \frac{c_i^2}{i!} (X^{s_i})^\top X^{s_i} \right) \leq \sum_{i=2}^{\infty} \frac{c_i^2}{i!} \sigma_{\max} (X^{s_i}) \leq c_\infty^2 \sigma_{\max}^2 (X) \tag{A.36}$$

where $c_\infty$ is given by

$$c_\infty^2 = \sum_{i=2}^{\infty} \frac{c_i^2}{i!},$$
which is finite provided that $||\phi||_{\mathcal{H}}$ is bounded.

Using (A.36), we now establish an upper bound on $\sigma_{\text{max}}(E[\tilde{M}_0])$:

$$\sigma_{\text{max}}(E[\tilde{M}_0]) \lesssim d_1 \left( n \sigma_0^2 + (\epsilon_1^2 + \epsilon_\infty^2) \sigma_{\text{max}}^2(X) \right).$$

Moreover, suppose there exists some $t$ such that $\sigma_{\text{min}}(X^{*t}) > 0$. This requires to have $d_0^t \geq n$.

Putting together the lower bound on $\sigma_{\text{min}}(E[\tilde{M}_0])$ and the upper bound on $\sigma_{\text{min}}(E[\tilde{M}_0])$, noting $W_0 = \omega_1 W_0^0$ and applying $\tau^\epsilon \phi(a) \leq \phi(\tau a) \leq \tau^\epsilon \phi(a)$, we have

$$\omega_1^{2r_1} d_1 \frac{c_0^2}{d_1!} \sigma_{\text{min}}^2(X^{*t}) \lesssim \sigma_{\text{min}}(E[\tilde{M}_0]) \leq \sigma_{\text{max}}(E[\tilde{M}_0]) \lesssim \omega_1^{2r_2} d_1 \left( n \sigma_0^2 + (\epsilon_1^2 + \epsilon_\infty^2) \sigma_{\text{max}}^2(X) \right).$$

(A.37)

### E.2 Concentration of the random matrix $M_0$

To see how well the random matrix $M_0$ concentrates about its expectation, note that

$$M_0 = \phi(X^\top W_0^\top) \phi(W_0 X) = \sum_{i=1}^{d_1} \phi(X^\top W_{0,i}^\top) \phi(W_{0,i} \to X) = \sum_{i=1}^{d_1} \tilde{A}_i$$

where $\{\tilde{A}_i\}_{i=1}^{d_1} \subset \mathbb{R}^{n \times n}$ are independent random matrices.

Consider the event $\mathcal{E}_1$ that

$$\max_{i \in [d_1]} \| W_{0,i} \to X \|_2 \lesssim k_1 \omega_1 \sqrt{d_0 \log d_1}, \quad \max_{i \in [d_1]} \| V_{0,i} \|_2 \lesssim k_2 \omega_2 \sqrt{d_2 \log d_1}$$

(A.39)

where $V_{0,i} \to X$ is the $i$-th column of $V_0$. Note that $W_{0,i} \to X \in \mathbb{R}^{d_0}$ and $V_{0,i} \in \mathbb{R}^{d_2}$ are random zero-mean Gaussian vectors whose entries’ variances are $\omega_1^2$ and $\omega_2^2$, respectively. Therefore, with an application of the scalar Bernstein inequality [6, Proposition 5.16], followed by the union bound, we observe that the event $\mathcal{E}_1$ happens except with a probability of at most

$$p_1 := d_1^{c k_1 d_0} + d_1^{c k_2 d_2},$$

(A.40)

for a universal constant $C$ with sufficiently large $k_1, k_2$.

Let $i \in [d_1]$. Conditioned on the event $\mathcal{E}_1$, an upper bound on $\| \phi(X^\top W_{0,i} \to X) \|_2$ is given by:

$$\| \phi(X^\top W_{0,i} \to X) \|_2 \lesssim \phi_{\max} \sigma_{\max}(X) k_1 \omega_1 \sqrt{d_0 \log d_1}.$$}

(A.41)

Moreover, we have

$$\sigma_{\max}(A_i) = \| \phi(X^\top W_{0,i} \to X) \|_2^2 = \| \phi(X^\top W_{0,i} \to X) - \phi(0) \|_2^2 \lesssim \phi_{\max}^2 \sigma_{\max}^2(X) k_1^2 \omega_1^2 d_0 \log d_1.$$  

(A.42)

We now focus on the concentration of $\sigma_{\min}(M_0)$ and $\sigma_{\max}(M_0)$. We use a concentration property, which provides the tail bound of $\hat{f}(W) = \phi(X^\top W^\top) \phi(W X)$ with multivariate Gaussian input $W$.

In the following lemma, we show that $\hat{f}$ is a Lipschitz function, and its Lipschitz constant explains how $\hat{f}(W)$ concentrates around its mean.

**Lemma A.3.** Let $\hat{f}(W) = \phi(X^\top W^\top) \phi(W X)$. Suppose $W$ satisfies (A.39). Then $\hat{f}$ is $\kappa$-Lipschitz function with constant $\kappa = 4 \phi_{\max}^2 \sigma_{\max}(X) k_1 \omega_1 \sqrt{d_0 \log d_1}$. So we have

$$\| \hat{f}(W) - \hat{f}(W') \| < 4 \phi_{\max}^2 \sigma_{\max}^2(X) k_1 \omega_1 \sqrt{d_0 \log d_1} \cdot \| W - W' \|.$$
Proof. Note that \( \tilde{f}(W_0) = M_0 \) and \( \tilde{f} \) can be represented as

\[
\tilde{f}(X) = \sum_{i=1}^{d_1} f_i(W_{i\to})
\]

where \( f_i \) is given by \( f_i(W_{i\to}) = \phi(X^TW_{i\to}^\top)\phi(W_{i\to}X) \). We prove that each \( f_i \) is \( \kappa \)-Lipschitz, which implies that \( \tilde{f} \) is also \( \kappa \)-Lipschitz.

We note that \( f_i \)'s can be expressed as a composition of three functions:

\[
\tilde{f}_i(v) = (g_1 \circ g_2 \circ g_3)(v)
\]

where \( g_1, g_2, \) and \( g_3 \) are given by

\[
g_1(v) = vv^\top, \quad g_2(v) = \phi(v), \quad g_3(v) = vX.
\]

(A.43)

It is clear that \( g_2 \) is \( \hat{\phi}_\text{max} \)-Lipschitz, and \( g_3 \) is \( \sigma_\text{max}(X) \)-Lipschitz from their definitions. Lipschitz constant of \( g_1 \) comes from the domain bound as follows:

\[
\|g_1(v + \delta v) - g_1(v)\| = \|\delta vv^\top + \delta v \delta v^\top\|
\]

\[
\leq 2\|\delta vv^\top\| + \|\delta v \delta v^\top\|
\]

\[
\leq (2\|v\| + \|\delta v\|)\|\delta v\|.
\]

(A.44)

A bound on \( (2\|v\| + \|\delta v\|) \) is obtained in (A.41). Then \( g_1 \) is \( \kappa_1 \)-Lipschitz function with \( \kappa_1 = 4\hat{\phi}_\text{max}\sigma_\text{max}(X)k_1\sqrt{d_0\log d_1} \). Therefore, all \( g_1, g_2 \), and \( g_3 \) are Lipschitz function, so their composition \( f_i \) is also Lipschitz function with constant \( \kappa = 4\hat{\phi}_\text{max}^2\sigma_\text{max}^2(X)k_1\sqrt{d_0\log d_1} \), which completes the proof.

Lemma A.4. Let \( z \in \mathbb{R}^d \) denote a Gaussian random vector. Then we have \( \Pr\{\|z - E[z]\| > t | \mathcal{E}_2\} \lesssim \exp(-t^2) \) where \( \mathcal{E}_2 \) is the event that \( \|z\| \) is bounded.

We can focus on the tail distribution of \( M_0 = \tilde{f}(W_0) \). Using Lemmas A.3 and A.4, we have

\[
\Pr\{\|M_0 - E[M_0]\| > t | \mathcal{E}_1\} \lesssim \exp(-k_2^2 t)
\]

(A.45)

where \( t = k_34\hat{\phi}_\text{max}^2\sigma_\text{max}^2(X)k_1\sqrt{d_0\log d_1} \) with some constant \( k_3 \).

Using (A.45), we now establish a tail bound on \( \sigma_{\text{min}}(M_0) \):

\[
\Pr\{\sigma_{\text{min}}(M_0) \leq (1 - \delta_1)\sigma_{\text{min}}(E[M_0]) | \mathcal{E}_1\} \leq \Pr\{\sigma_{\text{min}}(M_0) - E[M_0]) \geq \delta_1\sigma_{\text{min}}(E[M_0]) | \mathcal{E}_1\}
\]

\[
\leq \Pr\{\sigma_{\text{min}}(M_0) - E[M_0]) \geq \delta_1\sigma_{\text{min}}(E[M_0]) | \mathcal{E}_1\}
\]

\[
\leq \Pr\{\sigma_{\text{max}}(M_0 - E[M_0]) \geq \delta_1\sigma_{\text{min}}(E[M_0]) | \mathcal{E}_1\}
\]

\[
\leq \Pr\{\|M_0 - E[M_0]\| \geq \delta_1\sigma_{\text{min}}(E[M_0]) | \mathcal{E}_1\}
\]

\[
\lesssim p_2
\]

where

\[
p_2 = \exp\left(-\left(\frac{\delta_1\sigma_{\text{min}}(E[M_0])}{4\hat{\phi}_\text{max}^2\sigma_\text{max}^2(X)k_1\omega_1\sqrt{d_0\log d_1}}\right)^2\right).
\]

Similarly, we obtain

\[
\Pr\{\sigma_{\text{max}}(M_0) \geq (1 + \delta_2)\sigma_{\text{max}}(E[M_0]) | \mathcal{E}_1\} \lesssim p_3
\]

where

\[
p_3 = \exp\left(-\left(\frac{\delta_2\sigma_{\text{max}}(E[M_0])}{4\hat{\phi}_\text{max}^2\sigma_\text{max}^2(X)k_1\omega_1\sqrt{d_0\log d_1}}\right)^2\right).
\]

Putting these bounds together with (A.37), we have:

\[
\omega_1^{t_1}(1 - \delta_1)^{t_2}d_1\sigma_{\text{min}}(X^{t_1}) \leq \sigma_{\text{min}}(\phi(W_0X))
\]

(A.46)

\[
\sigma_{\text{max}}(\phi(W_0X)) \leq \sqrt{(1 + \delta_2)\omega_1^{t_2}(\sqrt{c_1^2 + c_2^2}d_1\sigma_{\text{max}}(X) + |c_0|\sqrt{d_1n})}
\]

except with a probability of at most \( p_1 + p_2 + p_3 \).

With establishing the bounds on \( \sigma_{\text{min}}(\phi(W_0X)) \) and \( \sigma_{\text{max}}(\phi(W_0X)) \), we can finally estimate \( \mu_\Phi, \nu_\Phi \) as follows:
E.3 Lower bound on $\mu_\Phi$

A lower bound on $\mu_\Phi$ is given by

$$
\omega_1^{*1} \sqrt{\frac{(1 - \delta_1) c_1^2}{t l}} d_1 \sigma_\text{min}(X^{*l}) \leq \sigma_\text{min}(\phi(W_0X)) = \mu_\Phi,
$$

(A.47)

except with a probability of at most $p_1 + p_2$.

E.4 Upper bound on $\nu_\Phi$

Since $\nu_\Phi = \hat{\sigma}_\text{max}(X)\sigma_\text{max}(V_0) + \sigma_\text{max}(\phi(W_0X))$, we obtain a bound on $\sigma_\text{max}(V_0)$:

$$
\sigma_\text{max}(V_0) \leq \omega_2 (2 \sqrt{d_1} + \sqrt{d_2}) \lesssim \omega_2 \sqrt{d_1},
$$

(A.48)

except with a probability of at most $p_4 = \exp(-C d_1)$ where $C$ is a universal constant [6][Corollary 5.35].

Combining (A.48) with the upper bound on $\sigma_\text{max}(\phi(W_0X))$, we have

$$
\nu_\Phi = \hat{\sigma}_\text{max}(X)\sigma_\text{max}(V_0) + \sigma_\text{max}(\phi(W_0X))
$$

$$
\lesssim \omega_2 \hat{\sigma}_\text{max}(X) \sqrt{d_1} + \omega_1^{*2} \sqrt{(1 + \delta_2) (c_1^2 + c_2^2 \delta_1) d_1 \sigma_\text{max}(X) + \omega_1^{*2} |\nu_2| \sqrt{(1 + \delta_2) d_1 n}}
$$

except with a probability of at most $p_1 + p_3 + p_4$.

E.5 Upper bound on $h(\Theta_0)$

In this section, we bound $h(\Theta_0)$. Using $\|a + b\|_2^2 \leq 2\|a\|_2^2 + 2\|b\|_2^2$, we have

$$
h(\Theta_0) = \|V_0\phi(W_0X) - Y\|^2
$$

$$
\leq 2\|V_0\phi(W_0X)\|^2 + 2\|Y\|^2.
$$

(A.49)

To upper bound the random norm in (A.49), we first decompose $V_0\phi(W_0X)$ into terms including $W_{0,i,\to} \in \mathbb{R}^{d_0}$ and $V_{0,i,\downarrow} \in \mathbb{R}^{d_2}$ as follows:

$$
V_0\phi(W_0X) = \sum_{i=1}^{d_1} B_i
$$

(A.50)

where $B_i = V_{0,i,\downarrow} \phi(W_{0,i,\to}^T X) \in \mathbb{R}^{d_2 \times n}$'s are independent random matrices for $i \in [d_1]$.

Conditioned on the event $E_1$ defined in (A.39), we bound $\|B_i\|:

$$
\|B_i\| = \|V_{0,i,\downarrow}\|_2 \|\phi(W_{0,i,\to}^T X)\|_2
$$

$$
\leq \|V_{0,i,\downarrow}\|_2 \cdot \hat{\sigma}_\text{max}(X) k_1 d_0 \sqrt{d_1 \log d_1}
$$

$$
\leq \omega_1 \hat{\sigma}_\text{max}(X) k_1 k_2 \sqrt{d_0 d_2 \log d_1}
$$

(A.51)

for $i \leq d_1$.

Substituting the upper bound in A.50 into A.51 and applying the Hoeffding inequality [2], we have

$$
\Pr\left\{\|V_0\phi(W_0X)\| \gtrsim u(d_0, d_1, d_2) |E_1\right\} = \Pr\{|\|V_0\phi(W_0X) - \mathbb{E}[V_0\phi(W_0X)]|\| \gtrsim u(d_0, d_1, d_2) |E_1\right\}
$$

$$
\leq \Pr\left\{\sum_{i=1}^{d_1} \|B_i - \mathbb{E}[B_i]\| \gtrsim u(d_0, d_1, d_2) |E_1\right\}
$$

$$
\leq p_5
$$

where

$$
u(d_0, d_1, d_2) = \delta_3 \omega_1 \omega_2 \hat{\sigma}_\text{max}(X) k_1 k_2 \sqrt{d_0 d_1 d_2 \log d_1}
$$

11
and $p_5 = \exp(-C\delta_3^2)$ with $\delta_3 \geq 0$ and a universal constant $C$.

Therefore, under the event $\mathcal{E}_1$, we have

$$h(\Theta_0) \leq 2\|V_0\phi(W_0X)\|^2 + 2\|Y\|^2 \leq \delta_2^2\omega_1^2\omega_2^2\phi_{\max}^2k_1^2k_2^2d_0d_1d_2\sigma_{\max}^2(X)\log^2 d_1 + \|Y\|^2$$  \hspace{1cm} (A.52)

except with a probability of at most $p_1 + p_5$. It is natural to assume that $d_2 = o(d_1)$. We also have $\|Y\| \leq 1$.

Suppose that

$$\omega_1\omega_2 \leq \frac{1}{\phi_{\max}\sqrt{d_0d_1\log d_1}}.$$  \hspace{1cm} (A.53)

Substituting (A.53) into (A.52), we have

$$h(\Theta_0) \leq \delta_2^2\omega_1^2\omega_2^2\phi_{\max}^2k_1^2k_2^2\sigma_{\max}^2(X)$$  \hspace{1cm} (A.54)

where $\delta_3$, $k_1$, and $k_2$ are all constants and independent of $d_0$, $d_1$, and $n$.

### E.6 Denouement

The key condition for linear rate convergence of gradient descent in (9) is

$$h(\Theta_0) \leq \frac{\alpha_f\mu_\Phi^6}{\beta_\Phi^2 k_\Phi^2}.$$  \hspace{1cm} (A.55)

Putting everything together for the shallow neural network, with high probably, we have

$$\alpha_f = 2$$

$$\nu_\Phi = \omega_2\phi_{\max}\sigma_{\max}(X)\sqrt{d_1} + \sqrt{(1 + \delta_2)\omega_1^2\sigma_{\max}(X)}\sqrt{d_1} + |c_0|\sqrt{\omega_1^2d_1n}$$

$$\mu_\Phi = \omega_1^2\sqrt{(1 - \delta_1)c_1^2 d_1}\sigma_{\min}(X^{*t})$$

$$\beta_\Phi = \sqrt{2}\sigma_{\max}(X)(\phi_{\max} + \phi_{\max}\chi_{\max}).$$  \hspace{1cm} (A.55)

We note that the order of $\sigma_{\max}(X)$ and $\sigma_{\min}(X^{*t})$ play significant roles for the overparameterization order analysis. For $t = 1$, it requires $n \approx d_0$, which is not a common setting in practice. In the following, we focus on $t \geq 2$.

### E.7 Order analysis with $t \geq 2$

In this section, we assume $|c_0|$ is sufficiently large such that $|c_0|\sqrt{1 + \delta_2}d_1n$ becomes the dominating term in $\nu_\Phi$.\footnote{To have a nonzero $c_0$, the activation function should not be an odd function.} Then a sufficient condition to satisfy (9) is

$$d_1^2 \geq \frac{\delta_3^2c_0^2(1 + \delta_2)k_1^2k_2^2(\phi_{\max} + \phi_{\max}\chi_{\max})^2\sigma_{\max}^2(X)n t^3}{\omega_1^{1 - 2r_2}c_1^{3\delta}\sigma_{\min}^2(X^{*t})}.$$  \hspace{1cm} (A.56)

which can be written as

$$d_1 \geq \sqrt{\frac{\delta_3^2c_0^2(1 + \delta_2)k_1^2k_2^2(\phi_{\max} + \phi_{\max}\chi_{\max})^2t^3}{\omega_1^{1 - 2r_2}c_1^{3\delta}}}.\frac{\sqrt{n}\sigma_{\max}(X)}{\sigma_{\min}^2(X^{*t})}.$$  \hspace{1cm} (A.56)

For notational simplicity, we let $\delta_4 = \max\{k_1, k_2\}$ and denote $\mathcal{C}_\delta = \{\delta_1, \delta_2, \delta_3, \delta_4\}$ and

$$\xi(c_\delta, t, \phi, \{c_i\}_{i \geq 0}) = \sqrt{\frac{\delta_3^2c_0^2(1 + \delta_2)\delta_4^2(\phi_{\max} + \phi_{\max}\chi_{\max})^2t^3}{\omega_1^{1 - 2r_2}c_1^{3\delta}}}.\frac{\sqrt{n}\sigma_{\max}(X)}{\sigma_{\min}^2(X^{*t})}.$$  \hspace{1cm} (A.57)
Note that \( \xi(C_\delta, t, \phi, \{c_i\}_{i \geq 0}) \) can be viewed as a constant w.r.t. \( d_0, d_1, \) and \( n \). Then (A.56) can be written as:

\[
d_1 = \tilde{\Omega}(\sqrt{n} \sigma_{\max}^2(X) / \sigma_{\min}^2(X^{*t})).
\]

It remains to estimate \( \sigma_{\max}(X) \) and \( \sigma_{\min}(X^{*t}) \) to finish the order analysis of \( d_1 \). Suppose that \( n \approx d_0 \).

Then, along the lines of [4][Section 2.1], we have \( \sigma_{\max}(X) \approx \sqrt{\frac{n}{d_0}} \) and \( \sigma_{\min}(X^{*t}) \approx \sqrt{\frac{n}{d_0}} \approx 1 \).

Combining them all, we have

\[
d_1 \gtrsim \xi(C_\delta, t, \phi, \{c_i\}_{i \geq 0}) \frac{n^{\frac{3}{2}}}{d_0}.
\]

Therefore, the overall overparameterization degree becomes \( d_0d_1 \approx \tilde{\Omega}(n^{\frac{3}{2}}) \) for \( t \geq 2 \).

The exact expression of \( \psi(\phi, \xi, d_0, d_1, d_2, X) \) in Theorem 3 is given by

\[
\psi \leq p_1 + p_2 + p_3 + p_4 + p_5
\]

\[
\leq d_1^{-C\delta_5d_0} + d_1^{-C\delta_4d_2} + e^{-\left(\frac{\delta_4}{\sigma_{\max}(\Theta^{(k)}M_0)}\right)^2} + e^{-\left(\frac{\delta_4}{\sigma_{\max}(\Theta^{(k)}M_0)}\right)^2} + e^{-C\delta_4} + e^{-C\delta_5^2}.
\]

Note that \( d_1^{-C\delta_5d_0} + d_1^{-C\delta_4d_2} + \exp(-C\delta_4) + \exp(-C\delta_5^2) \) decreases exponentially, which can be sufficiently small without changing the order of \( d_1 \).

Finally, with \( d_0d_1 \approx \tilde{\Omega}(n^{\frac{3}{2}}) \), the gradient descent converges to a global minimum with linear rate with probability at least \( 1 - \psi \), which can be arbitrary small.

**Order analysis without boundedness assumption on \( \sigma_{\max}(V_k) \) in Assumption 2.**

So far, we assumed \( \sigma_{\max}(V_k) \) is bounded for \( k \geq 0 \). We can relax this assumption by bounding the length of the trajectory of gradient descent as discussed in Appendix C. Recall (A.12):

\[
\ell(I) \approx \frac{\nu_\phi \sqrt{f(Z_0)}}{\sqrt{\alpha f^2} \mu_\Phi^2}.
\]

Using triangular inequality and substituting (A.12), we can obtain a bound on \( \|V_k\| \)

\[
\|V_k\| \leq \|V_k - V_0\| + \|V_0\|
\]

\[
\leq \frac{\nu_\phi \sqrt{f(Z_0)}}{\sqrt{\alpha f^2} \mu_\Phi^2} + \|V_0\|
\]

As shown in (A.48), \( \|V_0\| \leq \omega_2 \sqrt{d_1} \) with high probability over the choice of \( V_0 \). With sufficiently small \( \omega_2 \), the first term in the upper bound dominates in (A.60). Applying (A.54) and substituting (A.60) into (A.56), we have

\[
d_1 \gtrsim \frac{n^2 \sigma_{\max}^0(X)}{\sigma_{\min}^{10}(X^{*t})}
\]

\[
d_1 \gtrsim \frac{n^{\frac{3}{2}}}{d_0}.
\]

The overall overparameterization degree becomes \( d_0d_1 \approx \tilde{\Omega}(n^{\frac{3}{2}}) \), which is slightly worse than the result of Theorem 3 under boundedness assumption on \( \sigma_{\max}(V_k) \). Note that we still have a subquadratic scaling on the network width.

**F Additional discussion on lazy training in Section 6**

In this section, we provide an asymptotic analysis for the term \( \|h(\Theta_k) - \tilde{h}(\Theta_k)\| \) to show that there exists a regime where our initialization can avoid lazy training. Recall our setting:

\[
\Phi(\Theta) = V \cdot \phi(WX)
\]
where $W \sim \mathcal{N}(0, \omega_1^2)$ and $V \sim \mathcal{N}(0, \omega_2^2)$. Following the theoretical guidance in (19), we set
\[ \omega_1 \omega_2 \simeq \frac{1}{\sqrt{\omega_0 d_t}}. \]

An upper bound on $\|h(\Theta_i) - \tilde{h}(\Theta_i)\|$ is given by [1, Theorem 2.3]:
\[ \|h(\Theta_i) - \tilde{h}(\Theta_i)\| \leq \frac{\text{Lip}(\nabla \Phi(\Theta))}{\text{Lip}(\Phi(\Theta))^2}. \] (A.61)

In the following, we estimate $\frac{\text{Lip}(\nabla \Phi(\Theta))}{\text{Lip}(\Phi(\Theta))^2}$ to find when it is not bound to be close to zero.

Substituting $\beta_\Phi$ and $\nu_\Phi$ expressions in (A.55) into the upper bound in (A.61) for sufficiently large $n, c_0$, we have
\[ \|h(\Theta_i) - \tilde{h}(\Theta_i)\| \leq \sqrt{2} \sigma_{\max}(X) (\hat{\phi}_{\max} + \hat{\phi}_{\max} \chi_{\max}) \left( \frac{\omega_2 \phi_{\max} \sigma_{\max}(X) \sqrt{d_1} + \omega_1^2 c_0 \sqrt{(1 + \delta_2) d_1 n}}{(\omega_1^2 \phi_{\max} \sigma_{\max}(X) \sqrt{d_1} + \omega_1^2 c_0 \sqrt{(1 + \delta_2) d_1 n})^2} \right). \] (A.62)

We now find an upper bound on $\chi_{\max}$ by bounding the total length of the trajectory of gradient descent as in Appendix C where the length of the trajectory traced by gradient descent is given by (A.12):
\[ \ell(I) \leq \frac{\nu_\Phi \sqrt{f(Z_0)}}{\sqrt{\alpha_f \mu_\Phi^2}}. \]

Using (A.12), (A.48), and (A.54), a bound on $\chi_{\max}$ is given by
\[ \|V_i\|_2 \leq \|V_i - V_0\|_F + \|V_0\|_2 \]
\[ \leq \frac{\nu_\Phi \sqrt{f(Z_0)}}{\sqrt{\alpha_f \mu_\Phi^2}} + \|V_0\|_2 \]
\[ \leq \left( \frac{\omega_2 \phi_{\max} \sigma_{\max}(X) + \omega_1^2 c_0 \sqrt{n}) \sigma_{\max}(X)}{\omega_1^2 \sqrt{d_1} \sigma_{\min}(X^{*t})} + \omega_2 \sqrt{d_1} \right). \] (A.63)

Therefore we have
\[ \|h(\Theta_i) - \tilde{h}(\Theta_i)\| \leq \sqrt{2} \sigma_{\max}(X) \left( \hat{\phi}_{\max} + \hat{\phi}_{\max} \frac{(\omega_2 \phi_{\max} \sigma_{\max}(X) + \omega_1^2 c_0 \sqrt{n}) \sigma_{\max}(X)}{\omega_1^2 \sqrt{d_1} \sigma_{\min}(X^{*t})} + \omega_2 \phi_{\max} \sqrt{d_1} \right) \]
\[ \left( \frac{(\omega_2 \phi_{\max} \sigma_{\max}(X) \sqrt{d_1} + \omega_1^2 c_0 \sqrt{(1 + \delta_2) d_1 n})^2}{(\omega_1^2 \phi_{\max} \sigma_{\max}(X) \sqrt{d_1} + \omega_1^2 c_0 \sqrt{(1 + \delta_2) d_1 n})^2} \right). \]

We now consider two cases: 1) $\omega_2 \phi_{\max} \sigma_{\max}(X) \gtrsim \omega_1^2 c_0 \sqrt{n}$ and 2) $\omega_2 \phi_{\max} \sigma_{\max}(X) \lesssim \omega_1^2 c_0 \sqrt{n}$.

More precisely, for the asymptotic analysis, we consider extremal cases $\omega_1 \gg \omega_2$ and $\omega_1 \ll \omega_2$ and evaluate $\|h(\Theta_i) - \tilde{h}(\Theta_i)\|$ in each case:

**F.1 Regime with $\omega_2 \gg \omega_1$**

In the overparameterization regime with large $d$, we note that
\[ \hat{\phi}_{\max} \left( \frac{\omega_2 \phi_{\max} \sigma_{\max}(X) \sigma_{\max}(X)}{\omega_1 \sqrt{d_1} \sigma_{\min}(X^{*t})} \right) + \omega_2 \phi_{\max} \sqrt{d_1} \gtrsim \hat{\phi}_{\max}. \]

Then we have
We note that this upper bound above goes to $\infty$ in the regime $\omega_2 \gg \omega_1$, which means that gradient descent can avoid lazy training. Note that it does not imply this training scheme is guaranteed to be non-lazy though.

**F.2 Regime with $\omega_1 \gg \omega_2$**

In this regime, we have

$$\phi_{\text{max}} \left( \frac{\omega_2 \phi_{\text{max}} \sigma_{\text{max}}(X) + \omega_1^2 \phi_{\text{max}} \sqrt{n}}{\omega_1 \sqrt{d_1} \sigma_{\text{min}}(X^{*t})} \right) \ll \phi_{\text{max}} + \omega_2 \phi_{\text{max}} \sqrt{d_1}.$$  \hspace{1cm} (A.64)

Then we have

$$\|h(\Theta_t) - \tilde{h}(\Theta_t)\| \lesssim \frac{\sqrt{2} \sigma_{\text{max}}(X) \left( \frac{\phi_{\text{max}} + \omega_2 \phi_{\text{max}} \sqrt{d_1}}{\omega_2 \phi_{\text{max}} \sigma_{\text{max}}(X) \sqrt{d_1} + \omega_1^2 \phi_{\text{max}} \sigma_{\text{min}}(X^{*t})} \right)}{(\omega_2 \phi_{\text{max}} \sigma_{\text{max}}(X) \sqrt{d_1} + \omega_1^2 \phi_{\text{max}} \sigma_{\text{min}}(X^{*t}))^2}.$$  \hspace{1cm} (A.64)

Note that this bound goes to 0 and lazy training is bound to happen asymptotically.

**G Implementation details of Section 6**

For the experiments illustrated in Figure 1, we computed the training and test accuracy for different variants of the proposed weight initialization scheme. We considered the MNIST data set made available through the torchvision implementation\(^2\). We used the provided split of 60 000 training examples and 10 000 test examples which we subsequently normalized.

First, a teacher neural network was train on this data set. The label provided by the teacher was then used to relabel both the training and test examples. For each of the weight initializations a student network was constructed and trained on the relabeled data set. The student neural network had 1 000 units in its hidden layer and used the GeLU activation function. For the loss we used the mean square error against a one-hot encoding of the true class label. We minimized this loss with stochastic gradient descent (SGD) for which there was three hyperparameter choices. As the difficult of the data set was modest we expected a large range of these hyperparameters to work. It thus sufficed to make a reasonable guess by choosing a batch size of 128, learning rate of 0.01 and 300 epochs. The teacher neural network differed from the student network by using He initialization and cross entropy loss.

All results were implemented in PyTorch [5] and run on a Slurm cluster using a Tesla K40c GPU. We fixed $\omega_1/\omega_2 \approx 0.002259$ based on the He initialization for our particular network and varied $\omega_2$ in the range $[0.002, 0.1]$. We considered 10 different initialization in this range and ran 5 experiments for each configuration of weight initialization, $(\omega_1, \omega_2)$. Using these independent runs we plotted the mean and standard deviation of the final training and test accuracy in Figure 1, in Section 6.

\(^2\)This implementation uses the original MNIST source: \url{http://yann.lecun.com/exdb/mnist/}.
References


