Abstract

We prove that two-layer (Leaky)ReLU networks initialized by e.g. the widely used method proposed by He et al. [2015] and trained using gradient descent on a least-squares loss are not universally consistent. Specifically, we describe a large class of data-generating distributions for which, with high probability, gradient descent only finds a bad local minimum of the optimization landscape. It turns out that in these cases, the found network essentially performs linear regression even if the target function is non-linear. We further provide numerical evidence that this happens in practical situations and that stochastic gradient descent exhibits similar behavior.

1 Introduction

In recent years, neural networks (NNs) have achieved various success stories in areas such as image classification, sentiment analysis, and speech recognition. For this reason, NNs are commonly viewed as one of the state-of-the-art machine learning algorithms. Unlike for other machine learning algorithms, however, our theoretical understanding of their learning behavior, e.g. in terms of a-priori learning guarantees, is still rather limited.

Probably the simplest of such a-priori guarantees is the notion of universal consistency, see e.g. the books by [Devroye et al. 1996, Györfi et al. 2002], that demands the population risk of the learned model to converge to the smallest possible population risk as the number of samples goes to infinity. For simple learning methods such as histogram rules, kernel regression, and $k$-nearest neighbor rules, universal consistency has already been shown in the late 20th century, as outlined in the two books mentioned above.

In contrast, the situation is more difficult for neural networks, despite the fact that there do exist some consistency results for certain classes of NNs, see e.g. [White 1990] for regression, [Faragó and Lugosi 1993] for classification, and the books mentioned above for a broader overview. However, these results require an under-parameterized regime, in which the number of hidden neurons grows more slowly than the sample size, as well as a training algorithm that finds a global minimum. Unfortunately, finding a global minimum for small network sizes can be NP-hard, see e.g. the classical paper by [Blum and Rivest 1989] as well as [Boob et al. 2018], who establish similar results for certain ReLU-networks. Moreover, [Safran and Shamir 2018] have empirically shown that the probability of finding a bad local minimum in certain two-layer ReLU NNs with gradient descent (GD) can increase with increasing numbers of samples and neurons. Consequently, it remains possible that the consistency results mentioned above only apply to computationally infeasible NN training algorithms. On the other hand, a consistent NN training algorithm does not necessarily need to find a global optimum, and hence it also remains an open question whether practical NN algorithms such as variants of (stochastic) GD are consistent in the under-parameterized regime.

Based on the empirical observations in [Zhang et al. 2016], it has been more recently shown that finding a global minimum for over-parameterized NNs, i.e. for NNs whose number of neurons (significantly) exceeds the number of samples, is easier. For example, [Arora et al. 2018] present a poly-time algorithm for finding a global minimum for NNs with one hidden layer and [Mücke and Steinwart 2019] present such a training algorithm for NNs with two hidden layers. However, both algorithms are not based on (stochastic) GD. By imposing rather mild assumptions on the dataset, [Du et al. 2019a,b, Allen-Zhu et al. 2019] show that (stochastic) GD also reaches a global optimum with high probability. While these papers address the optimization problem of NNs, they do not provide guarantees such as consistency. In fact, [Mücke and Steinwart 2019] show...
that over-parameterized NNs of sufficient size always have both global minima with good generalization performance in the sense of consistency and global minima with very bad generalization performance. However, their global minima are more interesting from a theoretical point of view. Moreover, Zhang et al. [2016, Belkin et al. 2018] discuss in detail why common techniques from statistical learning theory cannot work for the analysis of over-parameterized NNs. Finally, Arora et al. [2019] present a generalization bound for certain ReLU-NNs with one hidden layer that involves a novel complexity measure in terms of a Gram matrix of a neural tangent kernel. However, this result is only stated for a special class of noise-free data-generating distributions.

In summary, it thus seems fair to say that neither positive nor negative a-priori guarantees for common NN training algorithms such as (stochastic) GD have been established.

In this paper, we address this lack of understanding in the following way: We prove that training under-parameterized ReLU or LeakyReLU networks with one hidden layer using GD on a least-squares loss does not yield an universally consistent estimator if e.g. the common initialization method by He et al. [2015] is used. Moreover, we prove that there also exist a multitude of data sets for which over-parameterized versions of such NNs cannot be properly trained by gradient descent. Empirical investigations further show that stochastic gradient descent has the same shortcomings.

This paper is an improved version of the first author’s master’s thesis [Holzmüller, 2019].

2 NN Architecture and Training

In this section we present the considered network architecture, the initialization, and the training process. For simplicity, we will mostly focus on one-dimensional inputs, but show in Remark 5 that our results for one-dimensional inputs can be easily generalized to multi-dimensional inputs.

Definition 1. Let \( \varphi : \mathbb{R} \to \mathbb{R} \) be the LeakyReLU function with fixed parameter \( \alpha \in \mathbb{R} \setminus \{\pm 1\} \), that is

\[
\varphi(x) := \begin{cases} 
  x & ,x \geq 0 \\
  \alpha x & ,x \leq 0
\end{cases}.
\]

We consider two-layer single-input single-output neural networks with \( m \in \mathbb{N} \) hidden neurons. Such a neural network defines a function \( f_W : \mathbb{R} \to \mathbb{R} \) via

\[
f_W(x) := c + \sum_{i=1}^{m} w_i \varphi(a_i x + b_i),
\]

where \( W = (a, b, c, w) \in \mathbb{R}^{3m+1} \) with \( a, b, w \in \mathbb{R}^m \) and \( c \in \mathbb{R} \). Note that \( \varphi \) is piecewise linear with a kink (non-differentiable point) at 0, and therefore the function \( f_W \) is piecewise affine linear with potential kinks at \( -b_i/a_i \).

Assumption 2. The components of the initial vector \( W_0 \) are initialized independently with distributions

\[
b_{i,0} = 0, \quad c_0 = 0, \quad a_{i,0} \sim Z_a, \quad w_{i,0} \sim \frac{1}{\sqrt{m}} Z_w,
\]

where \( Z_a, Z_w \) are \( \mathbb{R} \)-valued random variables satisfying:

\[
\text{(Q1)} \quad Z_a, Z_w \text{ have symmetric (even) and bounded probability density functions } p_a, p_w : \mathbb{R} \to [0, B_Z^a],
\]

\[
\text{(Q2)} \quad \mathbb{E}|Z_a|^p < \infty \text{ and } \mathbb{E}|Z_w|^p < \infty \text{ for all } p \in (0, \infty).
\]

We denote the distribution of \( W_0 \) by \( P_0^{\text{init}} \).

Importantly, Assumption 2 is satisfied by the initialization method of [He et al. 2015], where \( Z_a, Z_w \sim \mathcal{N}(0, 2) \). Our assumption is also satisfied for e.g. uniform distributions.

Definition 3. For a bounded distribution \( P \) on \( \mathbb{R} \times \mathbb{R} \), a dataset \( D = ((x_1, y_1), \ldots, (x_n, y_n)) \in (\mathbb{R} \times \mathbb{R})^n \), a weight vector \( W \in \mathbb{R}^{3m+1} \), and a (measurable) function \( f : \mathbb{R} \to \mathbb{R} \), we define the (least-squares) loss and risk by

\[
L_P(W) := R_P(f_W), \quad R_P(f) := \frac{1}{2} \mathbb{E}_{(x,y) \sim P} (y - f(x))^2,
\]

\[
L_D(W) := R_D(f_W), \quad R_D(f) := \frac{1}{2n} \sum_{j=1}^{n} (y_j - f(x_j))^2.
\]

Let \( P_X \) be the distribution of the \( x \) component of \( P \).

Definition 4. For \( m, n \in \mathbb{N} \), step size \( h > 0 \), \( P_m^{\text{init}} \) as in Assumption 2 and a dataset \( D \in (\mathbb{R} \times \mathbb{R})^n \), training the neural network produces a random sequence of functions \( (f_{W_k})_{k \in \mathbb{N}_0} \) via initializing \( W_0 \sim P_m^{\text{init}} \) and applying GD, i.e.

\[
W_{k+1} := W_k - h \nabla L_D(W_k).
\]

Remark 5 (Multi-dimensional input). We show in Appendix II that NNs with multi-dimensional input behave similarly in the following sense: For a fixed \( z \in \mathbb{R}^d \) with \( \|z\|_2 = 1 \) and \( D \) as above, consider the dataset \( \tilde{D} := ((x_1 z, y_1), \ldots, (x_n z, y_n)) \in (\mathbb{R}^d \times \mathbb{R})^n \). If we extend the definitions of \( L_D \) and \( f_W \), naturally to

\[
\text{by a bounded distribution on } \mathbb{R} \times \mathbb{R}, \text{ we mean a probability distribution } P \text{ for which there exists a bounded set } \Omega \subseteq \mathbb{R} \times \mathbb{R} \text{ with } P(\Omega) = 1. \text{ While we use bounded data distributions for simplicity, our proofs only use the finiteness of moments, i.e. the weaker assumption } f(\|x\|^p + |y|^p) \, dP(x,y) < \infty \text{ for all } p \in (0, \infty).
$d$-dimensional inputs, then for every random variable $\tilde{W}_0$, there exists a corresponding random variable $W_0$ such that the GD iterates

$$\tilde{W}_{k+1} = \tilde{W}_k - h\nabla L_D(\tilde{W}_k),$$
$$W_{k+1} = W_k - h\nabla L_D(W_k)$$

satisfy

$$f_{\tilde{W}_k}(xz) = f_{W_k}(x).$$

for all $x \in \mathbb{R}, k \in \mathbb{N}_0$. Moreover, if $\tilde{W}_0$ is initialized analogous to Assumption 2, then $W_0$ satisfies Assumption 2. In other words, if we have a dataset where all $x_j$ lie on a line $\text{Span}\{z\} \subseteq \mathbb{R}^d$, then an NN on the $d$-dimensional input space behaves on this line like an NN with one-dimensional input space.

3 A Closer Look at the Training Behavior

In this section we illustrate why the combination of zero bias initialization (which is the default in TensorFlow and Keras) and GD training as may produce poorly predicting NNs. In the subsequent sections we then rigorously prove that such training behavior does occur with high probability.

Our first, rather basic observation is that zero bias initialization $b_i,0 = 0$ and $c_0 = 0$ as in Assumption 2 places all kinks $-b_i,0/a_{i,0}$ of the initial $f_{W_0}$ at zero. Consequently, $f_{W_0}$ is linear on both $(-\infty, 0]$ and $[0, \infty)$. In contrast, the function to be learned is typically nonlinear on these two sets, and finding a suitable NN approximation during training may thus require to substantially move at least some of the kinks. To illustrate this statement, consider Figure 1 in which a data set that requires a nonlinear predictor is depicted. It is obvious from Figure 1 that any reasonable NN approximation requires at least a few kinks in both $[-4, -1.5]$ and $[1.5, 4]$. The training algorithm thus needs to move a few kinks from 0 into these two areas. Unfortunately, such a behavior can in general not be guaranteed. For example, Figure 2 illustrates that on the data set $D$ of Figure 1, GD does not move the kinks outside the interval $[-0.2, 0.2]$ and in particular, no kink is moved across a sample, since no $x$-component of a sample of $D$ falls inside $[-0.5, 0.5]$. As a consequence, the corresponding NN predictors $f_{W_k}$, for $k \geq 1$, remain affine linear on the left part $D_{-1}$ and the right part $D_1$ of the data set $D$, as Figure 1 illustrates. This problem has been observed experimentally by Steinwart [2019], who suggests to use a data-dependent initialization method that places kinks randomly across all data points.

A closer look at Figure 1 further indicates that $f_{W_k}$ approaches the optimal affine linear regression lines for the two data sets $D_{-1}$ and $D_1$ with increasing $k$. As a consequence, GD gets stuck in a bad local minimum of the loss surface. Note that the existence of structurally similar bad local minima has already been shown in Yun et al. [2019], but there it remained an open question whether GD can avoid such bad minima. In the following sections, we rigorously show that under some assumptions on $D$ or $P$, on the stepsize $h$, and on $n$ and $m$, the predictors $f_{W_k}$ produced by GD remain affine linear on the negative and positive parts of $D$ with high probability. Consequently, GD does not escape from the corresponding bad local minima in such situations.

Figure 1: A dataset with $n = 300$ samples (black crosses), a close-to-optimal NN predictor (green line, kinks marked as circles) with $m = 16$, and functions $f_{W_k}$ for $k = [1.1^l] - 1, l \in \{0, \ldots, 120\}$, $m = 16$, $h = 0.002$, trained on the visualized dataset. The colors of $f_{W_k}$ transition from blue to red to yellow, i.e. the lower blue function is $f_{W_0}$ and the upper red line is reached at an intermediate stage before the NN converges to the prominent yellow line.

Figure 2 also shows that the kinks initially move very fast but then slow down. Empirically, this slowdown is related to the loss, whose evolution relative to the reached optimum in our example is also shown in Figure 2. In our theoretical analysis, we find that the convergence of the neural network and the movement of the kinks are related to a four-dimensional linear iteration equation. Here, the system matrix has two eigenvalues of order $-\Theta(m)$ leading to a fast convergence and two eigenvalues of order $-\Theta(1)$ leading to a slow convergence. In the example of this section, the initialization of this system is close to the fast eigenvectors, which leads to the two-step decay of the loss in Figure 2.
Figure 2: This figure shows the evolution of several quantities during training in Figure 1. The thick red line shows $L_D(W_k) - \inf_{k' \in \mathbb{N}_0} L_D(W_{k'})$, where the latter infimum is the minimal loss that can be reached by fitting $D_1$ and $D_{-1}$ with linear regression similar to the yellow line in Figure 1. The thin black lines show the 16 NN kinks in Figure 1 (one can see only 14 kinks since there are two almost identical pairs of paths). The right y-axis in this plot corresponds to the x-positions of the kinks in Figure 1. The initial fast movement happens within approximately 100 epochs.

4 Main Result

Before we can state the main result of our work, we need to introduce some more notions.

Definition 6. For given data set $D$, the subsequence of samples $(x_j, y_j)$ with $x_j > 0$ is denoted by $D_1$. Analogously, $D_{-1}$ denotes the samples with $x_j < 0$. Moreover, for a distribution $P$, we define the measures $P_1$ and $P_{-1}$ via

$$P_1(E) := P(E \cap (0, \infty) \times \mathbb{R})$$

$$P_{-1}(E) := P(E \cap ((-\infty, 0) \times \mathbb{R}))$$

With the help of $D_{\pm 1}$ and $P_{\pm 1}$ we now define the “linear regression optima”, which will be crucial for our analysis.

Definition 7. For $P$ and $D$ as in Definition 3, $x, y \in \mathbb{R}$, and $\sigma \in \{\pm 1\}$, we define

$$M_x := \begin{pmatrix} x^2 & x \\ x & 1 \end{pmatrix}, \quad \tilde{u}_{(x,y)} := \begin{pmatrix} xy \\ y \end{pmatrix}$$

$$M_{D,\sigma} := \frac{1}{n} \sum_{(x,y) \in D_\sigma} M_x, \quad \tilde{u}_{D,\sigma} := \frac{1}{n} \sum_{(x,y) \in D_\sigma} \tilde{u}_{(x,y)}$$

$$M_{P,\sigma} := \int M_x dP_\sigma(x,y), \quad \tilde{u}_{P,\sigma} := \int \tilde{u}_{(x,y)} dP_\sigma(x,y).$$

Moreover, if the $2 \times 2$ matrix $M_{D,\sigma}$ is invertible, we write

$$\psi_{opt} := \begin{pmatrix} p_{opt} \\ q_{opt} \end{pmatrix} := M_{D,\sigma}^{-1} \tilde{u}_{D,\sigma}.$$

Note that $p_{D,\sigma}^\text{opt}$ and $q_{D,\sigma}^\text{opt}$ are the slope and intercept of the optimal linear regression line for $D_\sigma$, see Remark D.5 for a proof and Figure D.2 for an illustration.

In the sequel, we are mostly interested in the maximal absolute slopes and intercepts as well as the distance of $D$ to 0, i.e.

$$\psi_{D,\sigma} := \max \left\{ |p_{D,\sigma}^\text{opt}|, |q_{D,\sigma}^\text{opt}| \right\},$$

$$\psi_D := \max \left\{ |q_{D,1}^\text{opt}|, |q_{D,-1}^\text{opt}| \right\},$$

$$\Delta_D := \min \{|x_1|, \ldots, |x_n|\}.$$ If $M_{P,\sigma}$ is invertible, the quantities $\psi_{P,\sigma}^\text{opt}, q_{P,\sigma}^\text{opt}$, $p_{P,\sigma}$, and $\psi_D$ are defined and interpreted analogously. Finally, the smallest and the largest eigenvalue of a symmetric matrix $A$ are denoted by $\lambda_{\text{min}}(A)$ and $\lambda_{\text{max}}(A)$.

Throughout this work, we require $D_1$ and $D_{-1}$ to be non-empty. However, it is also possible to prove analogous results for the cases where $D$ or $P^{\text{data}}$ are solely concentrated on $(-\infty, 0)$ or $(0, \infty)$, cf. Remark D.4.

We can now state our main theorem, which is proven at the end of Appendix G. In Theorem 10 and Theorem 19, we then apply this main theorem to over-parameterized and under-parameterized NNs, respectively.

Theorem 8. Let $\varepsilon > 0$ and let $\gamma_\psi, \gamma_{\text{data}}, \gamma_P \geq 0$ with $\gamma_\psi + \gamma_{\text{data}} + \gamma_P < 1/2$. Then, for given $K_{\text{data}}, K_\psi, K_M > 0$, there exist $C_P, C_{lr}, C_{\text{weights}} > 0$ such that the following statement holds:

For all neural networks with width $m \in \mathbb{N}$ and step size $h > 0$, and all data sets $D$ satisfying

(a) $K_M^{-1} \leq \lambda_{\text{min}}(M_{D,\pm 1}) \leq \lambda_{\text{max}}(M_{D,\pm 1}) \leq K_M$

(b) $\psi_{D,\sigma} \leq K_\psi$

(c) $\psi_{D,\sigma} \leq K_\psi m_{\gamma_\psi}^{-1}$

(d) $\Delta_D \geq K_{\text{data}} m_{\gamma_{\text{data}}}^{-1}$

(e) $h \leq C_h m_{\gamma_{\text{data}}}^{-1}$

the random training sequence $(f_{W_k})_{k \in \mathbb{N}_0}$ has the following properties with probability $\geq 1 - C_P m_{\gamma_P}^{-\varepsilon}:

(i) For all $i$, $|a_{i,k} - a_{i,0}| \leq C_{\text{weights}} m_{\gamma_\psi + \varepsilon}^{-3/2}$.

(ii) For all $i$, $|b_{i,k} - b_{i,0}| \leq C_{\text{weights}} m_{\gamma_\psi + \varepsilon}^{-3/2}$.

(iii) For all $i$, $|w_{i,k} - w_{i,0}| \leq C_{\text{weights}} m_{\gamma_\psi + \varepsilon}^{-1}$.

(iv) For all $i$, $|c_{i,k} - c_{i,0}| \leq C_{\text{weights}} m_{\gamma_\psi + \varepsilon}^{-1}$.

(v) For all $k \in \mathbb{N}_0$, $f_{W_k}$ is affine on the intervals $(-\infty, -K_{\text{data}} m_{\gamma_{\text{data}}}^{-1})$ and $(K_{\text{data}} m_{\gamma_{\text{data}}}^{-1}, \infty)$.

Remark 9. The data-independent condition (e) involves a conservative constant $C_{\text{weights}}$. In Proposition F.4 and the proof of Theorem 8, we show that (e) can be replaced by $h \leq \lambda_{\text{max}}(H)^{-1}$, where $H \in \mathbb{R}^{4 \times 4}$ is a symmetric positive (semi-)definite matrix, which is defined in Definition F.1 and which can be computed from $D$ and $W_0$. ▲
Theorem 8 states that if $D$ is inside certain bounds and the step size $h$ is sufficiently small, the NN function $f_{W_k}$ remains affine on $D_1$ and $D_{-1}$ with high probability and the weights $W_k$ do not change much. This behavior is independent of when the iteration is stopped. In the following, we will examine when the assumptions on $D$ are satisfied.

5 Over-parameterization

The following theorem considers a fixed dataset $D$ of arbitrary size $n$ and arbitrary network widths $m$. In particular, it applies to the over-parameterized case $m > n$.

Theorem 10. Let $D$ be fixed such that $M_{D,\pm 1}$ are invertible and $\psi_{D,q} = 0$. Let $\varepsilon > 0$ and let $\gamma_{\text{data}}, \gamma_P \geq 0$ with $\gamma_{\text{data}} + \gamma_P < 1/2$. Then, there exist $C_P, C_{\text{lr}}, C_{\text{weights}} > 0$ such that the following statement holds:

For all widths $m \in \mathbb{N}$ and all step sizes $0 < h \leq C_{\text{lr}}^{-1} m^{-1}$, the random sequence $(f_{W_k})_{k \in \mathbb{N}_0}$ satisfies (i) – (v) in Theorem 8 with $K_{\text{data}} = \mathbb{E} D$ with probability $\geq 1 - C_P m^{-\gamma_P}$.

Proof. Under the assumptions of Theorem 10, we can choose $\gamma_{\psi} = 0$, $K_{\text{data}} = \mathbb{E} D$, and $K_{\psi}, K_M$ suitably large such that the assumptions of Theorem 8 are satisfied. By Theorem 8 we then obtain constants $C_{\text{lr}}, C_P, C_{\text{weights}} > 0$ such that the conclusions of the theorem hold.

Lemma J.1 shows that for one-dimensional $D$ with $x_j \neq 0$ for all $j$, the assumptions on $D$ can always be satisfied by adding three more points to $D$. By Theorem 10 these points can play the role of adversarial training samples.

Example 11. Let $m \in \mathbb{N}$ be large and $D$ be the dataset

$$((-3, -1), (-2, 2), (-1, -1), (1, 1), (2, -2), (3, 1)).$$

Then, $M_{D,\sigma}$ is invertible for $\sigma \in \{\pm 1\}$ and $u^0_{D,\pm 1} = 0$ implies $\psi_{D,q} = 0$. Theorem 10 thus shows that with high probability $f_{W_k}$ is affine linear on $[1, \infty)$ and $(-\infty, -1]$ for all $k \geq 1$, and hence the $f_{W_k}$’s do not interpolate $D$. GD does therefore not come even close to a global optimum.

6 Inconsistency

In this section we describe a class of bounded distributions that produce data sets satisfying the assumptions of Theorem 8 with high probability. To describe the failure of GD in this case, we need to recall the following classical notion from statistical learning, see e.g. Steinwart and Christmann [2008].

Definition 12. A learning method, i.e. a method that produces for each dataset $D$ a potentially random predictor $f_D$, is called consistent for a bounded distribution $P_{\text{data}}$, if for all $\varepsilon > 0$, the probability of sampling a dataset $D$ with $n$ i.i.d. samples $(x_j, y_j) \sim P_{\text{data}}$ satisfying

$$R_{\text{plata}}(f_D) \geq R^*_{\text{plata}} + \varepsilon$$

covers 0 as $n \to \infty$, where $R^*_{\text{plata}}$ is the optimal risk, i.e. $R^*_{\text{plata}} \equiv \inf_{f : \mathbb{R} \to \mathbb{R}} R_{\text{plata}}(f)$. The learning method is universally consistent if this holds for all such $P_{\text{data}}$.

Roughly speaking, universally consistent learning methods are guaranteed to produce close-to-optimal predictors for $n \to \infty$, independently of the data generating distribution $P_{\text{data}}$. Universal consistency is therefore widely accepted as a minimal requirement for statistically sound learning methods, see e.g. Devroye et al. [1996].

Next we will show that NNs initialized and trained as in Section 2 are not universally consistent in a strong sense. Namely, we show that inconsistency occurs for all distributions satisfying the following assumption. For its formulation we denote the set of all $f : \mathbb{R} \to \mathbb{R}$ that are affine on both $(-\infty, 0)$ and $(0, \infty)$ by $F_0$.

Assumption 13. The bounded distribution $P_{\text{data}}$ satisfies:

(P1) For all $\sigma \in \{\pm 1\}$, $M_{\text{plata, }\sigma}$ is invertible.

(P2) For a fixed $\eta \in (4, \infty]$, we have

$$P_{\text{data}}\left([-x, x]\right) = O(x^{\eta}) \quad \text{for } x \searrow 0, \quad (\eta < \infty)$$

$$P_{\text{data}}\left([-\delta, \delta]\right) = 0 \quad \text{for some } \delta > 0. \quad (\eta = \infty)$$

(P3) The intercepts of Definition 7 satisfy $\psi_{\text{plata, }q} = 0$.

(P4) We have $\inf_{f \in F_0} R_{\text{plata}}(f) > R^*_{\text{plata}}$.

The next remarks show, e.g. that $P_{\text{data}}$ satisfies (P1) and (P2), if the distribution $P_{\text{data}}$ of the $x$ component has a density that is sufficiently small around 0. They further show that we can always enforce (P3) and that (P4) means that the target function to be learned is not affine linear in the sense of $F_0$. As an example, note that the dataset in Figure 1 is sampled from a distribution satisfying Assumption 13.
Remark 14. (P1) is satisfied if $P^\text{data}_\sigma((\mathbb{R} \setminus \{x\}) \times \mathbb{R}) > 0$ for all $x \in \mathbb{R}$. Indeed, the kernel of the matrix $M_x$ is $\text{Span}\{1, -x\}^\top$, and hence there is, for any vector $\mathbf{v} \neq \mathbf{0} \in \mathbb{R}^2$, at most one $x \in \mathbb{R}$ with $\mathbf{v}^\top M_x \mathbf{v} = 0$. This gives
\[ \mathbf{v}^\top M_{\text{data},\sigma} \mathbf{v} = \int \mathbf{v}^\top M_x \mathbf{v} dP^\text{data}_\sigma(x, y) > 0. \]
In particular, (P1) is satisfied if e.g., $P^\text{data}_\sigma$ has a density that does not vanish on $(-\infty, 0] \cup [0, \infty)$.

Remark 15. (P2) holds if e.g. $P^\text{data}_X$ has a density $p$ with
\[ p(x) = O(|x|^\eta - 1) \quad \text{for} \quad x \to 0, \quad (\eta < \infty) \]
\[ p(x) = 0 \quad \text{for} \quad x \in (-\delta, \delta) \text{ for some} \quad \delta > 0. \quad (\eta = \infty) \]

Remark 16. Let $P^\text{data}$ be a bounded distribution satisfying (P1), (P2), and (P4), and let us fix a pair of random variables $(X, Y) \sim P^\text{data}$. Then the distribution $P^\text{data}$ of the vertically shifted random variables $(X, Y - y^\text{opt}_{\text{data,sgn}(X)})$ satisfies Assumption 13.

Remark 17. Recall from e.g. Steinwart and Christmann [2008] that the risk $R^\text{data}_\sigma$ is minimized by the conditional expectation $f^*(x) = E_{P^\text{data}}(Y|X)$ and that the excess risk of a predictor $f : \mathbb{R} \to \mathbb{R}$ is
\[ R^\text{data}_\sigma(f) - R^\text{data}_\sigma = \int |f(x) - f^*(x)|^2 dP^\text{data}_\sigma(x). \]
(P4) thus states that the least squares target function $f^*$ cannot be approximated by essentially affine functions.

The next proposition, whose proof is delegated to Proposition E.5, helps us to show that the assumptions of Theorem 8 are satisfied when sampling $D$ from $P^\text{data}$. In its formulation we use the convention $\infty \cdot 0 := \infty$.

Proposition 18. Let $P^\text{data}$ satisfy (P1) – (P3) from Assumption 13 let $\varepsilon, K_{\text{data}} > 0$, $m \geq 1$ and $\gamma_{\text{data}}, \gamma' \geq 0$. If $\eta = \infty \geq 0$ we further assume that $K_{\text{data}}$ satisfies $P^\text{data}_\sigma((-K_{\text{data}}, K_{\text{data}}) \times \mathbb{R}) = 0$. Finally, let $D$ be a dataset with $n$ data points $(x_j, y_j)$ sampled independently from $P^\text{data}$. Then with probability $1 - O(n^{-\gamma'} + n\eta^{-\gamma_{\text{data}}})$ the following hold:
\begin{enumerate}[(D1)]
    \item $\|v^{\text{opt}}_D - v^{\text{opt}}_{\text{data}}\|_{\infty} \leq \varepsilon n^{-1/2}$,
    \item For $\sigma \in \{\pm 1\}$, $\frac{1}{2}\lambda_{\min}(M_{\text{data},\sigma}) \leq \lambda_{\min}(M_{D,\sigma})$ and $\lambda_{\max}(M_{D,\sigma}) < 2\lambda_{\max}(M_{\text{data},\sigma})$,
    \item $\varepsilon_D \geq K_{\text{data}} n^{-\gamma_{\text{data}}}.$
\end{enumerate}
By combining Proposition 18 with Theorem 8 we obtain the following theorem.

Theorem 19. Let $P^\text{data}$ satisfy Assumption 13 let $\varepsilon > 0$, and let $\gamma_{\psi}, \gamma_{\text{data}}, \gamma_P \geq 0$ with $\gamma_{\psi} + \gamma_{\text{data}} + \gamma_P < 1/2$. Then, for given $K_{\text{param}}, K_{\text{data}} > 0$, where $K_{\text{data}}$ needs to satisfy $P^\text{data}_\sigma((-K_{\text{data}}, K_{\text{data}}) \times \mathbb{R}) = 0$ if $\eta = \infty$, there exist $C_P, C_{\text{lr}}, C_{\text{weights}} > 0$ such that the following statement holds:

For all $n \geq 1$, all widths $m \in \mathbb{N}$, all step sizes $h$ with
\[ 0 < h \leq C_{\text{lr}} m^{-1} \]
\[ m \leq K_{\text{param}} n^{1-2\gamma_{\psi}}, \]
and datasets $D$ with $n$ independent $(x_j, y_j) \sim P^\text{data}$, the random sequence $(f^{\text{data}}_k)_{k \in \mathbb{N}_0}$ satisfies (i) – (v) of Theorem 8 with probability not less than $1 - C_{P}(m^{-\gamma_P} + nm^{-\gamma_{\text{data}}})$.

Proof. Let $\bar{\varepsilon} > 0$ be small enough such that $\gamma_{\psi} := 2\bar{\varepsilon} + \gamma_{\psi}$ satisfies $\gamma_{\psi} + \gamma_{\text{data}} + \gamma_P < 1/2$. Under the assumptions above, there is a constant $K_M > 0$ such that for any dataset $D$ satisfying (D1) – (D3), we have
\[ \frac{1}{K_M} \leq \lambda_{\min}(M_{D,\pm1}) \leq \lambda_{\max}(M_{D,\pm1}) \leq K_M \]
\[ \left\| v^{\text{opt}}_D - v^{\text{opt}}_{\text{data}} \right\|_\infty \leq n^{(\frac{1}{2} - 1/2)} \leq O(m^{(2 - 2\gamma_{\psi})(\frac{1}{2} - 1/2)}) \]
\[ \leq O(m^{\frac{2}{2} + \gamma_{\psi} - 1}) = O(m^{\gamma_{\psi} - 1}). \]
It follows that
\[ \psi_{D,q} \leq \psi_{\text{data},q} + \left\| v^{\text{opt}}_D - v^{\text{opt}}_{\text{data}} \right\|_\infty \leq O(m^{\gamma_{\psi} - 1}) \]
\[ \psi_{D,p} \leq \psi_{\text{data},p} + \left\| v^{\text{opt}}_D - v^{\text{opt}}_{\text{data}} \right\|_\infty \leq O(m^{\gamma_{\psi} - 1}) \leq O(1). \]
Then, by Theorem 8 there exists $C_{\text{lr}} > 0$ such that (i) – (v) of Theorem 8 hold with probability $1 - O(m^{-\gamma_P})$ if $0 < h \leq C_{\text{lr}} m^{-1}$. Because of (P1) and (P2), Proposition 18 shows that the conditions (D1) – (D3) hold with probability
\[ 1 - O(n^{-\gamma'} + nm^{-\gamma_{\text{data}}}). \]
Here, $n^{-\gamma'} \leq O(m^{-\gamma_P})$ and $O(m^{-\gamma_P}) \leq O(m^{-\gamma_{\psi}})$ if we choose $\gamma' \geq \gamma_P$. By the union bound, the conclusions therefore hold with the specified probabilities.

Remark 20. A simple calculation shows that the condition $\eta > 4$ is necessary and sufficient for finding a sequence $m$ with $nm^{-\gamma_{\text{data}}}$ to 0 and $m \leq K_{\text{param}} n^{1-2\gamma_{\psi}}$.

The next two corollaries, whose proofs are given at the end of Appendix I, establish the announced inconsistency result for under-parametrized NNs. Appendix I further contains a generalization of Corollary 21 to the case $\eta < \infty$. 


Corollary 21. Consider the learning method that, given a $D \in (\mathbb{R} \times \mathbb{R})^n$, chooses a function $f_D = f_{W_k}$, where $k$ can be arbitrarily chosen. If $h_n < o(m^{-1})$, $\lim_{n \to \infty} m_n = 0$ and $m_n = O(n^{1-\varepsilon})$ for fixed $\varepsilon > 0$, then this learning method is not consistent for every $P_{\text{data}}$ satisfying Assumption 13 for $\eta = \infty$.

Corollary 22. Consider a learning method as in Corollary 21 but for $d$-dimensional data sets $D \in (\mathbb{R}^d \times \mathbb{R})^n$. Then this learning method is not universally consistent.

7 Proof idea

Here, we want to give an overview over the proof of Theorem 8. We omit technical terms with exponent $\varepsilon$ for simplicity and choose a different order than in the appendix.

As explained in Section 3, we want to show that the kinks $-b_{i,k}/a_{i,k}$ do not move much during training. For that, we want to show that $|a_{i,0}| \geq \Omega(m^{-1-\gamma})$ with probability $1 - O(m^{-\gamma})$. Hence, if $|a_{i,0}| < o(m^{-1-\gamma})$, then we still have $|a_{i,k}| \geq \Omega(m^{-1-\gamma})$. Moreover, if $|b_{i,k}| = |b_{i,k} - b_{i,0}| \leq O(m^{-1-\gamma}m_{\text{data}})$, then $|a_{i,k}| = O(m^{-\gamma}m_{\text{data}})$ and the main conclusion (v) of Theorem 8 follows.

Note that the (Leaky)ReLU $\varphi$ satisfies $\varphi(a_i x + b_i) = \varphi'(\text{sgn}(a_i x + b_i)) (a_i x + b_i)$. We then investigate GD on a modified loss function $L_{D_{\tau}}$, where we replace $\varphi'(\text{sgn}(a_i x + b_i))$ by $\varphi'(\text{sgn}(a_i x + b_i))$. If GD on this modified loss does not move the kinks much, then $\text{sgn}(a_i x + b_i)$ remains constant and $\nabla L_{D_{\tau}}(W_k) = \nabla L_{D}(W_k)$. On both loss functions GD will thus yield the same result. Such a strategy has also been used by Li and Liang 2018.

Next, we will explain how to bound the change in $b_{i,k}$, the situation for $a_{i,k}$ is analogous. One can show that with $\sigma := \text{sgn}(a_{i,0})$, we have $b_{i,k+1} = b_{i,l} + h w_{i,l} s_{\sigma,l}$ for a quantity $s_{\sigma,l}$ defined in Definition C.1. We can then derive

$$|b_{i,k} - b_{i,l}| \leq h \sum_{l=0}^{k-1} |w_{i,l} s_{\sigma,l}|$$

$$\leq \left( \sup_{0 \leq l < k} |w_{i,l}| \right) \cdot h \sum_{l=0}^{k-1} |s_{\sigma,l}|$$

$$\leq \left( |w_{i,0}| + \sup_{0 \leq l < k} |w_{i,l} - w_{i,0}| \right) \cdot h \sum_{l=0}^{k-1} |s_{\sigma,l}|.$$  \hspace{1cm} (1)

Given a bound on $h \sum_{l=0}^{k-1} |s_{\sigma,l}|$, bounding $|b_{i,k} - b_{i,l}|$ in this way requires bounding $|w_{i,l} - w_{i,0}|$. Bounding the latter with a similar argument would require bounding $|b_{i,l} - b_{i,0}|$ and so on. While one can proceed by proving bounds using induction, we resolve the problem in a different but similar fashion in Proposition C.2 which does not require guessing an induction hypothesis.

As mentioned before, the neural network functions $f_{W_k}$ are piecewise affine. Hence there are affine functions $f_{W_{k,1}}(x) = p_{1,k} x + q_{1,k}$ and $f_{W_{k,-1}}(x) = p_{-1,k} x + q_{-1,k}$ such that $f_{W_k}(x) = f_{W_{k,1}}(x)$ for sufficiently large $x > 0$ and $f_{W_k}(x) = f_{W_{k,-1}}(x)$ for sufficiently small $x < 0$. A central quantity in our proof is the vector

$$\tau_k := \begin{pmatrix} p_{1,k} - p_{D,1}^{\text{opt}} \\ p_{-1,k} - p_{D,-1}^{\text{opt}} \\ q_{1,k} - q_{D,1}^{\text{opt}} \\ q_{-1,k} - q_{D,-1}^{\text{opt}} \end{pmatrix}$$

containing the difference of the slope and intercept parameters to their affine regression optimum. We show in Appendix C that $s_{\sigma,l}$ is a linear combination of components of $\tau_k$. Thus, any bound on $h \sum_{l=0}^{k-1} |\tau_k|$ directly yields a bound on $h \sum_{l=0}^{k-1} |s_{\sigma,l}|$. We also show that

$$\tau_{k+1} = (I_4 - h A_k M_D ) \tau_k ,$$

where $A_k \in \mathbb{R}^{4 \times 4}$ depends on $W_k$ and $M_D \in \mathbb{R}^{4 \times 4}$ is assembled using $M_{D,1}$ and $M_{D,-1}$. Under the hypothesis that $W_k$ is close to $W_0$, we have $A_k \approx A^{\text{ref}}$, where $A^{\text{ref}} \in \mathbb{R}^{4 \times 4}$ is a suitable matrix only depending on $W_0$.

We first consider a reference system $\bar{v}_{k+1} = (I_4 - h A^{\text{ref}} M_D ) v_i$. It can be shown that $A^{\text{ref}}$ and $M_D$ are symmetric and positive definite (s.p.d.) with probability one. By a change of basis, we obtain the s.p.d. matrix $H = M_D^{1/2} A^{\text{ref}} M_D^{1/2} = M_D^{1/2} (A^{\text{ref}} M_D) M_D^{1/2}$. Hence, $A^{\text{ref}} M_D$ has positive real eigenvalues $\lambda_1, \ldots, \lambda_4$ with eigenvectors $v_1, \ldots, v_4$. If $\bar{v}_0 = \sum_{i=1}^{4} C_i v_i$, then

$$\bar{v}_k = \sum_{i=1}^{4} (1 - h \lambda_i)^k C_i v_i$$

and for $0 < h \leq (\max_i \lambda_i)^{-1}$, i.e. $1 - h \lambda_i \in [0, 1)$, we thus find

$$h \sum_{l=0}^{\infty} |\bar{v}_l| \leq \sum_{i=1}^{4} h \sum_{l=0}^{\infty} (1 - h \lambda_i)^l |C_i| \|v_i\|$$

$$= \sum_{i=1}^{4} \lambda_i^{-1} |C_i| \|v_i\| .$$

The idea is now to show that, with high probability, $\lambda_1, \lambda_2 = \Theta(m)$ and $\lambda_3, \lambda_4 = \Theta(1)$, while $\|v_i\| = O(1)$, $|C_1|, |C_2| = O(1)$ and $|C_3|, |C_4| = O(m^{\tau \cdot \omega^{-1}})$ in order to obtain the bound

$$h \sum_{l=0}^{\infty} |\bar{v}_l| \leq O(m^{\tau \cdot \omega^{-1}}) .$$
Indeed, we show in Proposition F.4 that \( \text{Span}\{v_1, v_2\} \approx \text{Span}\{e_1, e_2\} \) with the first two standard unit vectors \( e_1, e_2 \in \mathbb{R}^4 \). With \( q_{0,0} = 0 \) and \( \psi_{D,q} = O(m^{7\gamma - 1}) \), we also show that \( \bar{v}_0 \) is close to \( \text{Span}\{e_1, e_2\} \) and therefore \( |C_3|, |C_4| = O(m^{7\gamma - 1}) \).

In Proposition G.6 we perform an induction showing that \( W_k \) is close to \( W_0 \) and that the solution of \( \bar{v}_{k+1} = (I_4 - hA_k M_D)\bar{v}_k \) behaves similar to the solution of the reference system \( \bar{v}_{k+1} = (I_4 - hA_{\text{ref}} M_D)\bar{v}_k \). Inserting the result into Eq. (1) yields the asymptotics

\[
[b_{i,k} - b_{i,0}] = (O(m^{-1/2}) + o(m^{-1/2}))O(m^{7\gamma - 1}) = O(m^{7\gamma - 3/2}).
\]

By our assumption \( \gamma_{\psi} + \gamma_{\text{data}} + \gamma_P < 1/2 \), we have \( m^{7\gamma - 3/2} = o(m^{-1 - \gamma_{\text{data}} - \gamma_P}) \) and as outlined in the beginning of this section, all kinks only move by \( O(m^{-\gamma_{\text{data}}}) \).

The idea of deriving a system as in Eq. (2) and using induction to prove that \( W \) does not change much over time has already been used by e.g. [Du et al. 2019b].

The main novelties in this part of our proof are:

- In our scenario, we are able to use a four-dimensional system instead of a \( n \)-dimensional system.
- We find different eigenvalue asymptotics, which requires more sophisticated arguments to exploit.
- We prove different bounds on the change of weights in different layers, which is a consequence of using a more realistic parameterization of the NN. We also prove strong bounds on certain “second-moment” weight statistics, cf. Remark G.4.

8 Experiments

In this section, we present empirical evidence from Monte Carlo experiments that

1. the failure of kinks to move sufficiently far to reach data points can occur for realistic network sizes with high probability, and
2. SGD can exhibit a similar behavior when combined with an early stopping rule.

Data for the figures in this section can be reproduced using the code at

[github.com/dholzmueller/nn_inconsistency](https://github.com/dholzmueller/nn_inconsistency)

We use the following experimental setup: We compute each estimated probability using \( 10^4 \) Monte Carlo trials. We choose \( P_{\text{data}} \) as the uniform distribution on the dataset \( D \) from Example 11 and sample a dataset \( D' \) of size \( n = m^2 \) from \( P_{\text{data}} \). We then either use gradient descent or stochastic gradient descent (SGD) with batch size 16 in order to train the network and check whether a kink \( -b_{i,k}/a_{i,k} \) leaves the interval \((-1, 1)\), in which case we can stop training. For some experiments, we also stop training if an early stopping (ES) criterion is satisfied. For GD, we can also stop if the techniques used in Proposition F.4, Proposition G.2 and Proposition G.6 guarantee that no kink will ever leave \((-1, 1)\).

For the step size \( h \), unless specified otherwise, we use our maximal upper bound \( h = \lambda_{\text{max}}(H)^{-1} \) as mentioned in Remark 9 in order to reduce the number of iterations needed. We observe experimentally that \( \lambda_{\text{max}}(H)^{-1} \approx 0.4m^{-1} \) for our choice of \( P_{\text{data}} \).

Figure 3 shows how the probabilities behave as \( m \), and thus \( n = m^2 \), increases. In our scenario, we can apply Theorem 19 with \( \gamma_{\psi} = \gamma_{\text{data}} = 0 \) and obtain that the probabilities should behave like \( O(m^{-\gamma}) \) for all \( \gamma < 1/2 \). In Figure 3 this behavior can be observed even for small \( m \) and also for SGD.

As shown in 2 Ignoring the unlikely case \( a_{i,k} = 0, f_{u,i} \) remains affine on \(( -\infty, -1 ] \) and \([ 1, \infty ) \) if no kink leaves \([-1, 1]\).

3 We use early stopping as implemented in Keras [Chollet et al. 2015] with patience = 10 and min_delta = \( 10^{-8} \) Every 1000 epochs (GD) or 1000 batches (SGD), we monitor the loss on an independently drawn validation set of size \( n \). Whenever \( L_{\text{val}} < L_{\text{ref}} - 10^{-8} \), where \( L_{\text{val}} \) is the validation loss, we set \( L_{\text{ref}} := L_{\text{val}} \). Training is stopped when \( L_{\text{ref}} \) did not decrease within the last ten checks.

4 Without early stopping, SGD might still be able to move kinks far enough after a large number of iterations due to noisy gradients.
Figure 4: Monte-Carlo estimates ($10^4$ trials) of the probability of a kink crossing a sample for different values of $m, n = m^2$ using GD without early stopping. Here, the data distribution $P^{\text{data}}$ of Figure 3 is shifted upwards, i.e. in $y$-direction, by $\Delta$.

**Figure 2** kinks also move by significant amounts in later stages of the optimization. It is therefore not surprising that compared to considering $f_{W_k}$ for all $k \in \mathbb{N}_0$, using early stopping can significantly reduce the probability that a kink leaves $(-1, 1)$ during training. We see this especially for the small step size $h = 0.01m^{-1}$ in Figure 3. If we shift $P^{\text{data}}$ upwards by adding $\Delta \in \mathbb{R}$ to all $y$ values, we have $\psi_{P^{\text{data}}, \phi} = |\Delta|$ and assumption (P3) from Assumption 13 is violated. We can see in Figure 4 that this changes the asymptotic behavior, but for small $m$ and $|\Delta|$, the probabilities are still similarly low.

**9 Conclusion**

We have proven that NNs can fail with high probability in the over-parameterized regime for certain datasets and in the under-parameterized regime even for sampled datasets. In these cases, the NN converges to a local “linear regression” optimum. In particular, our analysis reveals that the difference of the NN to this linear regression optimum consists of a fast-decaying and a slow-decaying component and that for certain datasets, the slow-decaying component is already small at initialization. In essence, the reason is that learning is done mainly by the last layer, which contains $m$ weights but only one bias and therefore, the bias is learned more slowly than the weights. Especially, in our case, the NN operates in a “lazy regime” where the NN stays close to a “linearized version” around its initialization.

Using slightly different assumptions, Du et al. 2019b show convergence of over-parameterized NNs to a global minimum. One of their assumptions is that no two data points $x_i, x_j$ should be parallel. This assumption is violated in our scenario, where all $x_j$ are parallel. Ironically, the case where samples lie on a submanifold of the input space is often considered a strength of Deep Learning methods. Given such a dataset with parallel $x_j$, we can satisfy the assumption of Du et al. 2019b using $\tilde{x}_j := (x_j, 1)$. This corresponds to choosing $b_i \sim \mathcal{N}(0, 2)$ instead of $b_i = 0$, i.e. the kinks are now distributed randomly over $\mathbb{R}$. Consequently, given enough over-parameterization, there are already enough kinks available such that an NN could achieve zero training loss without moving them at all. Our paper shows that there are scenarios where kinks do not move much despite being initialized to a suboptimal place. This raises the question whether kinks move suitably in an intermediate case, e.g. if they are initialized randomly but the NN is not over-parameterized. It is also remains open whether our results can be generalized to deep NNs, other loss functions, or other optimization methods.

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\footnote{For example, they use no biases $b, c$ and they use the so-called NTK parameterization. The NTK parameterization is essentially equivalent to using a smaller learning rate for the second layer, which might lead to a different optimization result than the usual parameterization.}
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A Notation and Matrix Algebra

In this section, we will introduce some notation that is used throughout the appendix. We will also list some results about matrices, especially involving matrix norms and eigenvalues, cf. e.g. [Bhatia 2013], [Golub and Van Loan 1989].

Definition A.1. We denote the sign of a real number $x \in \mathbb{R}$ by

\[
\text{sgn}(x) = \begin{cases} 
1, & \text{if } x > 0 \\
0, & \text{if } x = 0 \\
-1, & \text{if } x < 0 .
\end{cases}
\]

For a set $S$, we denote its indicator function by $\mathbbm{1}_S$, i.e.

\[
\mathbbm{1}_S(x) = \begin{cases} 
1, & \text{if } x \in S \\
0, & \text{otherwise}.
\end{cases}
\]

Definition A.2 (Asymptotic notation). We use standard asymptotic notation $f \prec o(g), f \preceq O(g), f = \Theta(g), f \succeq \Omega(g)$ (we do not need $f > \omega(g)$). The constant in such an asymptotic (in)equality should not depend on

- the number $m$ of hidden neurons,
- the number $n$ of data points,
- the step size $h > 0$,
- step count variables such as $k, l, l' \in \mathbb{N}_0$,
- the initialization $W_0$,
- the dataset $D$,

as long as these variables satisfy the imposed assumptions. For example, we have $K_{\text{data}}m^{-\gamma_{\text{data}}} = \Theta(m^{-\gamma_{\text{data}}})$ for $K_{\text{data}} > 0$, but not $nm^{-\gamma_{\text{data}}} = O(m^{-\gamma_{\text{data}}})$. ▷

Definition A.3. Let $n, m \geq 1$, let $A, B \in \mathbb{R}^{m \times m}$ and $C \in \mathbb{R}^{n \times m}$. (We sometimes use $m, n$ to denote arbitrary vector space dimensions instead of numbers of hidden neurons and data points.)

1. We write $A > 0$ iff $A$ is symmetric and positive definite and $A \succeq 0$ iff $A$ is symmetric and positive semidefinite. We define $\preceq$ and $\prec$ analogously.

2. A symmetric matrix $A$ has an orthogonal eigendecomposition $A = UDU^\top$ with $U \in \mathbb{R}^{m \times m}$ orthogonal and $D \in \mathbb{R}^{m \times m}$ diagonal such that $D$ contains the (real) eigenvalues of $A$. We denote the set of eigenvalues of $A$ by $\text{eig}(A)$ and define

\[
\lambda_{\max}(A) := \max \text{eig}(A) \\
\lambda_{\min}(A) := \min \text{eig}(A).
\]

The matrix $A$ is invertible iff $0 \notin \text{eig}(A)$ and we have $A \succeq 0$ iff $\text{eig}(A) \subseteq [0, \infty)$. In the latter case, we can define the (symmetric) square root of $A$ as $A^{1/2} := U D^{1/2} U^\top$, where $D^{1/2}$ contains the square roots of the entries of $D$. Similarly, $A^{-1} = UD^{-1} U^\top$, which yields

\[
\lambda_{\max}(A^{1/2}) = \lambda_{\max}(A)^{1/2}, \quad \lambda_{\min}(A^{1/2}) = \lambda_{\min}(A)^{1/2}, \\
\lambda_{\max}(A^{-1}) = \lambda_{\min}(A)^{-1}, \quad \lambda_{\min}(A^{-1}) = \lambda_{\max}(A)^{-1}.
\]

3. As matrix norms, we use the Frobenius norm as well as the induced 2- and $\infty$-norms:

\[
\|C\|_F = \left( \sum_{i,j} C_{i,j}^2 \right)^{1/2}
\]

Sometimes, we also need to assume that $m, n$ is sufficiently large to be able to write $f \leq O(g)$ even if $f$ is infinite or undefined for small $m, n$. ▷
\[
\|C\|_2 = \sup_{x \neq 0} \frac{\|Cx\|_2}{\|x\|_2}
\]
\[
\|C\|_\infty = \sup_{x \neq 0} \frac{\|Cx\|_\infty}{\|x\|_\infty} = \max_i \sum_j |C_{ij}|
\]

If \( C \succeq 0 \), then \( \|C\|_2 = \lambda_{\text{max}}(C) \).

These matrix norms satisfy the following inequalities (cf. e.g. Section 2.3 in [Golub and Van Loan, 1989]):

\[
\|C\|_2 \leq \|C\|_F \leq \sqrt{m} \|C\|_2
\]
\[
\frac{1}{\sqrt{m}} \|C\|_\infty \leq \|C\|_2 \leq \sqrt{n} \|C\|_\infty
\]

Moreover, if \( C' \) is a subblock of \( C \), then \( \|C'\|_p \leq \|C\|_p \) for \( p \in \{2, F, \infty\} \).

(4) We define the condition number of a matrix \( A > 0 \) by

\[
\text{cond}(A) := \|A\|_2 \cdot \|A^{-1}\|_2 = \lambda_{\text{max}}(A) \lambda_{\text{min}}(A^{-1}) = \frac{\lambda_{\text{max}}(A)}{\lambda_{\text{min}}(A)}
\]

(5) We occasionally use element-wise operations on matrices. For example, \( |A| \) is the matrix containing as entries the absolute values of the entries of \( A \) and \( \sup_x A(s) \) consists of the element-wise suprema. Also, \( A \leq B \) means that \( A_{ij} \leq B_{ij} \) for all \( i, j \).

There are some more facts about matrices that we will use during some proofs. We show some typical arguments here:

- We will use the fact that for symmetric \( A \),

\[
\lambda_{\text{max}}(A) = \sup_{\|v\|_2 = 1} v^\top Av = \|A\|_2, \quad \lambda_{\text{min}}(A) = \inf_{\|v\|_2 = 1} v^\top Av,
\]

which is a special case of the Courant-Fischer-Weyl min-max principle (e.g. Corollary III.1.2 in [Bhatia, 2013]). This shows \( A \succeq 0 \Leftrightarrow \lambda_{\text{min}}(A) \geq 0 \). For \( A, B \succeq 0 \), we can use such an argument to show that

\[
\lambda_{\text{max}}(A + B) \leq \lambda_{\text{max}}(A) + \lambda_{\text{max}}(B)
\]
\[
\lambda_{\text{min}}(A + B) \geq \lambda_{\text{min}}(A) + \lambda_{\text{min}}(B)
\]

- If

\[
M = \begin{pmatrix} M_{11} & M_{12} \\ M_{12}^\top & M_{22} \end{pmatrix} \succeq 0,
\]

we know that

\[
x^\top M_{11} x = \begin{pmatrix} x \\ 0 \end{pmatrix}^\top M \begin{pmatrix} x \\ 0 \end{pmatrix} \geq \lambda_{\text{min}}(M) \|x\|_2^2 \geq 0,
\]

hence \( M_{11} \succeq 0 \) with \( \lambda_{\text{min}}(M_{11}) \geq \lambda_{\text{min}}(M) \). Similarly, \( \lambda_{\text{max}}(M_{11}) \leq \lambda_{\text{max}}(M) \) and analogous identities hold for \( M_{22} \). We also have

\[
\text{eig} \begin{pmatrix} M_1 & M_2 \\ M_2 \end{pmatrix} = \text{eig}(M_1) \cup \text{eig}(M_2) \quad \text{and therefore} \quad \begin{pmatrix} M_1 & M_2 \\ M_2 \end{pmatrix} > 0 \text{ iff } M_1, M_2 > 0.
\]

**B Gradient Descent with Fixed Activation Pattern**

In this section, we construct a modified loss function \( L_{D,T} \) which fixes the activation pattern of the neurons to its state at initialization. We also show that \( L_{D,T}(W) = L_D(W) \) for \( W \approx W_0 \) and introduce a shorter notation for gradient descent updates.
Definition B.1 (Fixed activation pattern). Define

\[ \tau_i := \text{sgn}(a_{i,0}) \]
\[ I := \{1, \ldots, m\} \]
\[ J := \{1, \ldots, n\} \]
\[ I_\sigma := \{ i \in I \mid \tau_i = \sigma \} \]
\[ J_\sigma := \{ j \in J \mid \text{sgn}(x_j) = \sigma \} \]
\[ f_{W,\tau,\sigma}(x) := c + \sum_{i \in I} w_i \varphi'(\sigma \tau_i) \cdot (a_i x + b_i) \]
\[ L_{D,\tau}(W) := \frac{1}{2n} \sum_{j \in J} (y_j - f_{W,\tau,\text{sgn}(x_j)}(x_j))^2. \]

The previous definition is motivated by the following lemma:

Lemma B.2. For \( \varphi > 0 \) and \( W_0 \in \mathbb{R}^{3m+1} \), consider the open set

\[ S_{W_0}(\varphi) := \{ W \in \mathbb{R}^{3m+1} \mid \forall i \in I : |b_i| < (|a_{i,0}| - |a_{i,0} - a_i|)\varphi \} . \]

The functions \( f_{W,\tau,\sigma} \) are affine and for all \( W \in S_{W_0}(\varphi) \) and all \( x \in \mathbb{R} \) with \( |x| \geq \varphi \), we have

\[ f_W(x) = f_{W,\tau,\text{sgn}(x)}(x) . \]

If \( \varphi_D > 0 \), we have

\[ L_D(W) = L_{D,\tau}(W), \quad \nabla L_D(W) = \nabla L_{D,\tau}(W) \]

for all \( W \in S_{W_0}(\varphi_D) \).

Proof. Trivially, \( f_{W,\tau,\sigma} \) is affine. Now, let \( W \in S_{W_0}(\varphi) \), let \( i \in I \) and let \( |x| \geq \varphi \). We then obtain that \( |a_{i,0} - |a_{i,0} - a_i| > 0 \) and therefore

\[ |b_i| < (|a_{i,0}| - |a_{i,0} - a_i|)|x| . \]

Since \( b_{i,0} = 0 \), we have

\[ |(a_i x + b_i) - (a_{i,0} x + b_{i,0})| \leq |a_i - a_{i,0}| \cdot |x| + |b_i| < |a_{i,0}| \cdot |x| = |a_{i,0} x + b_{i,0}| . \]

This shows \( \text{sgn}(a_i x + b_i) = \text{sgn}(a_{i,0} x + b_{i,0}) \), where

\[ \text{sgn}(a_{i,0} x + b_{i,0}) = \text{sgn}(a_{i,0}) \cdot \text{sgn}(x) = \tau_i \cdot \text{sgn}(x) . \]

Due to our special choice of \( \varphi \), we have

\[ \varphi(a_i x + b_i) = \varphi'(a_i x + b_i) \cdot (a_i x + b_i) = \varphi'(\text{sgn}(a_i x + b_i)) \cdot (a_i x + b_i) \]
\[ = \varphi'(\tau_i \cdot \text{sgn}(x)) \cdot (a_i x + b_i) , \]

which yields

\[ f_W(x) = f_{W,\tau,\text{sgn}(x)}(x) . \]

Since all datapoints \( x_j \) satisfy \( |x_j| \geq \varphi_D \) by definition of \( \varphi_D \), we find that

\[ L_{D,\tau}(W) = \frac{1}{2n} \sum_{j \in J} (y_j - f_{W,\tau,\text{sgn}(x)}(x_j))^2 = \frac{1}{2n} \sum_{j \in J} (y_j - f_W(x_j))^2 = L_D(W) . \]

In addition, because \( L_{D,\tau} \) and \( L_D \) are equal on the open set \( S_{W_0}(\varphi_D) \), their derivatives must also be equal on \( S_{W_0}(\varphi_D) \). □
We can now define gradient descent iterates with respect to the “linearized” loss function $L_{D,\tau}$.

**Definition B.3 (Gradient descent).** Given the random initial vector $W_0$, its activation pattern $\tau$ and a step size $h > 0$, we recursively define

$$W_{k+1} := W_k - h\nabla L_{D,\tau}(W_k).$$

Moreover, we write $W_k = (a_{-k}, b_{-k}, c_k, w_{-k})$ and we may implicitly omit the index $k$ when deriving identities that hold for each $k \in \mathbb{N}_0$. For any derived quantity $\xi := g(W)$, define

$$\delta \xi := \delta g(W) := g(W - h\nabla L_{D,\tau}(W)) - g(W)$$

such that

$$\xi_{k+1} = g(W_{k+1}) = g(W_k) + (g(W_{k+1}) - g(W_k)) = \xi_k + \delta \xi_k$$

and hence

$$\delta g(W) = g(W + \delta W) - g(W).$$

We can now write iteration rules differently: Instead of

$$W_{k+1} = W_k - h\nabla L_{D,\tau}(W_k),$$

we will use the more convenient notation

$$\delta W = -h\nabla L_{D,\tau}(W)$$

which suppresses the iteration index $k$ and reads more like the negative gradient flow ODE

$$\dot{W} = -h\nabla L_{D,\tau}(W).$$

The following lemma introduces some convenient rules for using $\delta$.

**Lemma B.4 (Differential calculus for $\delta$).** Let $g : \mathbb{R}^{3m+1} \to \mathbb{R}^N$ for some $m, N \geq 1$.

(a) If $g$ is linear, then $\delta g(W) = g(\delta W) = -hg(\nabla L_{D,\tau}(W)).$

(b) If $g$ is constant, then $\delta g = 0$.

(c) If $g_1, g_2 : \mathbb{R}^{3m+1} \to \mathbb{R}$ are linear, then

$$\delta (g_1 \cdot g_2) = (\delta g_1) \cdot g_2 + g_1 \cdot (\delta g_2) + (\delta g_1) \cdot (\delta g_2).$$

(d) If $g_1, g_2 : \mathbb{R}^{3m+1} \to \mathbb{R}^N$, then

$$\delta (g_1 + g_2) = \delta g_1 + \delta g_2.$$

(e) If $g_2 : \mathbb{R}^{3m+1} \to \mathbb{R}^N, g_1 : \mathbb{R}^N \to \mathbb{R}^{N'}$ and $g_1$ is linear, then

$$\delta (g_1 \circ g_2) = g_1 \circ (\delta g_2).$$

(f) If $g_1, \ldots, g_N : \mathbb{R}^{3m+1} \to \mathbb{R}$, then

$$\delta \begin{pmatrix} g_1 \\ \vdots \\ g_N \end{pmatrix} = \begin{pmatrix} \delta g_1 \\ \vdots \\ \delta g_N \end{pmatrix}.$$

**Proof.**

(a) If $g$ is linear, then

$$\delta g(W) = g(W + \delta W) - g(W) = g(\delta W) = g(-h\nabla L_{D,\tau}(W)) = -hg(\nabla L_{D,\tau}(W)).$$
(b) Trivial.

(c) In this case,
\[
\delta g(W) = g(W + \delta W) - g(W) = g_1(W)g_2(\delta W) + g_1(\delta W)g_2(W) + g_1(\delta W)g_2(\delta W) = \delta g_1(W)g_2(W) + g_1(W)\delta g_2(W) + \delta g_1(W)\delta g_2(W) .
\]

(d) We have
\[
\delta(g_1 + g_2)(W) = (g_1 + g_2)(W + \delta W) - (g_1 + g_2)(W) = (g_1(W + \delta W) - g_1(W)) + (g_2(W + \delta W) - g_2(W)) = \delta g_1(W) + \delta g_2(W) .
\]

(e) For \( W \in \mathbb{R}^{3n+1} \),
\[
\delta(g_1 \circ g_2)(W) = g_1(g_2(W + \delta W)) - g_1(g_2(W)) = g_1(g_2(W + \delta W) - g_2(W)) = g_1(\delta g_2(W)) .
\]

(f) This follows from
\[
\begin{pmatrix}
g_1 \\
\vdots \\
g_N
\end{pmatrix}(W + \delta W) - 
\begin{pmatrix}
g_1 \\
\vdots \\
g_N
\end{pmatrix}(W) = 
\begin{pmatrix}
g_1(W + \delta W) - g_1(W) \\
\vdots \\
g_N(W + \delta W) - g_N(W)
\end{pmatrix} .
\]

\[\square\]

C Reformulation of Gradient Descent

In this section, we will derive equations that describe how different aspects of the neural network behave during gradient descent. A summary and interpretation of the derived equations is presented in Appendix D.

**Definition C.1** (Derived quantities).

(a) For \( \sigma \in \{\pm 1\} \), we write \( \Sigma_{\sigma,a} := \sum_{i \in I_2} a_i^2 \), \( \Sigma_{\sigma,wa} := \sum_{i \in I_2} w_i a_i \) and so on.

(b) The matrix \( \mathbf{M}_\sigma := \mathbf{M}_{D,\sigma} \) from Definition 7 helps in relating different interesting quantities. For \( \mathbf{M}_\sigma > 0 \), let
\[
\mathbf{v}_\sigma := \begin{pmatrix}
\hat{p}_\sigma \\
\hat{q}_\sigma \\
\hat{r}_\sigma \\
\hat{s}_\sigma
\end{pmatrix} := \begin{pmatrix}
\Sigma_{\sigma,wa} \\
\Sigma_{\sigma,wb}
\end{pmatrix} \\
\mathbf{v}_\sigma := \begin{pmatrix}
p_\sigma \\
q_\sigma \\
r_\sigma \\
s_\sigma
\end{pmatrix} := \begin{pmatrix}
\hat{p}_\sigma + \alpha \hat{p}_{-\sigma} \\
\hat{q}_\sigma + \alpha \hat{q}_{-\sigma} \\
\hat{r}_\sigma + \alpha \hat{r}_{-\sigma} \\
\hat{s}_\sigma + \alpha \hat{s}_{-\sigma}
\end{pmatrix}
\]

and
\[
\mathbf{v}_\sigma := \mathbf{v}_\sigma - \mathbf{v}^{opt}_\sigma .
\]

We will show in Lemma C.4 that \( \hat{u}_\sigma = -\mathbf{M}_\sigma \mathbf{v}_\sigma \). The \( \mathbf{u} \)-vectors are interesting since their components can be used to simplify \( \delta W \). As we will see in Lemma C.4, \( \mathbf{v}_\sigma \) is interesting since \( f_{W,\tau,\sigma}(x) = p_\sigma x + q_\sigma \) for \( x \in \mathbb{R} \). The notation of the different variants is motivated as follows: Expressions with a hat such as \( \mathbf{v}_\sigma \) and \( \hat{u}_\sigma \) only sum over one sign \( \sigma \) while hat-less expressions include both \( \sigma = 1 \) and \( \sigma = -1 \).

We will also use the matrices
\[
G^w_\sigma := \begin{pmatrix}
\Sigma_{\sigma,wa} & 0 \\
0 & \Sigma_{\sigma,wb}
\end{pmatrix} , \quad G^{ab}_\sigma := \begin{pmatrix}
\Sigma_{\sigma,a} & \Sigma_{\sigma,ab} \\
\Sigma_{\sigma,ab} & \Sigma_{\sigma,b}
\end{pmatrix} , \quad G^{ab}_{\sigma} := (r_\sigma \Sigma_{\sigma,wa} + s_\sigma \Sigma_{\sigma,wb})I_2 ,
\]

where \( I_2 \) is the \( 2 \times 2 \) identity matrix.
(c) For any two vectors $z_1, z_{-1} \in \mathbb{R}^2$ defined in step (c) and any two matrices $F_1, F_{-1} \in \mathbb{R}^{2 \times 2}$ defined in step (b), we define

$$\tilde{z} := \begin{pmatrix} z_1 \\ z_{-1} \end{pmatrix} \in \mathbb{R}^4, \quad \tilde{F} := \begin{pmatrix} F_1 \\ F_{-1} \end{pmatrix} \in \mathbb{R}^{4 \times 4}.$$ 

For example, this means that

$$\tilde{u} = \begin{pmatrix} u_1 \\ u_{-1} \end{pmatrix} = \begin{pmatrix} r_1 \\ s_1 \\ r_{-1} \\ s_{-1} \end{pmatrix}.$$ 

In addition, we define new matrices

$$\tilde{C} := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}, \quad \tilde{B} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \alpha \\ \alpha & 0 & 1 & 0 \\ 0 & \alpha & 0 & 1 \end{pmatrix} = \begin{pmatrix} I_2 & \alpha I_2 \\ \alpha I_2 & I_2 \end{pmatrix},$$

$$\tilde{A} := \tilde{B}(\tilde{G}^w + \tilde{G}^{ab} + h\tilde{G}^{wab})\tilde{B} + \tilde{C}.$$ 

We will prove in Proposition C.5 that $\delta \tilde{v} = h\tilde{A}\tilde{u} = -h\tilde{A}\tilde{M}\tilde{v}$.

(d) We want to perform a change of basis using the permutation matrix $\tilde{P} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$, which satisfies $\tilde{P} = \tilde{P}^\top = \tilde{P}^{-1}$: For any vector $\tilde{z} \in \mathbb{R}^4$ and any matrix $\tilde{F} \in \mathbb{R}^{4 \times 4}$ defined in step (d), we define

$$z := \tilde{P}\tilde{z}, \quad F := \tilde{P}\tilde{F}\tilde{P}^{-1} = \tilde{P}\tilde{F}\tilde{P}.$$ 

For example, this yields

$$u = \tilde{P}\tilde{u} = \begin{pmatrix} r_1 \\ r_{-1} \\ s_1 \\ s_{-1} \end{pmatrix}, \quad C = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & \alpha & 1 \\ \alpha & 1 & 1 \\ 1 & \alpha & \alpha \end{pmatrix} =: \begin{pmatrix} \hat{B} \\ \hat{B} \end{pmatrix}.$$ 

We see that this change of basis by $\tilde{P}$ makes the matrices $\tilde{B}$ and $\tilde{C}$ block-diagonal while it destroys the block-diagonal structure of $\tilde{G}^{ab}$ and $\tilde{M}$. We will see in Lemma F.3 that $G^{ab}$ is still block-diagonal at initialization. We will use the tilde quantities as an intermediate step to derive equations for the non-tilde quantities, since the latter will be more suitable for us to analyze eigenvectors and eigenvalues.

Elementary arguments show that

$$(M_1 \succ 0 \text{ and } M_{-1} \succ 0) \Leftrightarrow \tilde{M} > 0 \Leftrightarrow M = \tilde{P}\tilde{M}\tilde{P}^\top > 0.$$ 

Therefore, we need to require $M > 0$ so that $v^{opt}$ and $\bar{v}$ can be defined.

(e) Many of the quantities above depend on the dataset $D$, which we may highlight later by indexing them with $D$. For example, we may write $u_D$ instead of $u$.

(f) Finally, let

$$\theta_i := \begin{pmatrix} a_i \\ b_i \\ w_i \end{pmatrix}, \quad \Sigma_{\sigma} := \sum_{i \in I_{\sigma}} \theta_i\theta_i^\top = \begin{pmatrix} \Sigma_{\sigma,a_2} & \Sigma_{\sigma,ab} & \Sigma_{\sigma,wa} \\ \Sigma_{\sigma,ab} & \Sigma_{\sigma,b^2} & \Sigma_{\sigma,wab} \\ \Sigma_{\sigma,wa} & \Sigma_{\sigma,wab} & \Sigma_{\sigma,w^2} \end{pmatrix}, \quad Q_{\sigma} := \begin{pmatrix} 0 & 0 & r_{\sigma} \\ 0 & 0 & s_{\sigma} \\ r_{\sigma} & s_{\sigma} & 0 \end{pmatrix}.$$ 

These quantities will be analyzed in the next proposition.
Proposition C.2. For \( i \in I_\sigma, \sigma \in \{\pm 1\} \), we have
\[
\delta \theta_i = hQ_\sigma \theta_i
\]
\[
\delta c = h(\hat{s}_1 + \hat{s}_{-1})
\]
\[
\delta \Sigma_\sigma = hQ_\sigma \Sigma_\sigma + h\Sigma_\sigma Q_\sigma + h^2 Q_\sigma \Sigma_\sigma Q_\sigma
\]
and the latter identity can also be written as
\[
\Sigma_{\sigma,k+1} = (I_3 + hQ_{\sigma,k})\Sigma_{\sigma,k}(I_3 + hQ_{\sigma,k})
\].

Proof. The first two equations can also be written as
\[
\delta a_i = hr_\sigma w_i
\]
\[
\delta b_i = hs_\sigma w_i
\]
\[
\delta w_i = hr_\sigma a_i + hs_\sigma b_i
\]
\[
\delta c = h(\hat{s}_1 + \hat{s}_{-1})
\].

We will prove the first of these equations, the other ones follow similarly. Set \( g(W) := a_i \). With Lemma B.4 (a), we obtain
\[
\delta a_i = \delta g(W) = -hg(\nabla L_{D,\tau}(W)) = -h\frac{\partial L_{D,\tau}}{\partial a_i}(W)
\]
\[
= -h\frac{1}{n} \sum_{j \in J} (f_{W,\tau,\text{sgn}(x_j)}(x_j) - y_j)\varphi'(\tau_i \cdot \text{sgn}(x_j))w_i x_j
\]
\[
= -h\frac{1}{n} \left( \sum_{j \in I_\sigma} (f_{W,\tau,\sigma}(x_j) - y_j)w_i x_j + \alpha \sum_{j \in J_{-\sigma}} (f_{W,\tau,-\sigma}(x_j) - y_j)w_i x_j \right)
\]
\[
= h(\hat{r}_\sigma + \alpha \hat{s}_{-\sigma})w_i = hr_\sigma w_i
\].

Now for \( \Sigma_\sigma \): Since \( Q_\sigma = Q_\sigma^T \), we have
\[
\Sigma_{\sigma,k+1} = \sum_{i \in I_\sigma} \theta_{i,k+1}^T \theta_{i,k+1} = \sum_{i \in I_\sigma} (I_3 + hQ_{\sigma,k})\theta_{i,k}^T (I_3 + hQ_{\sigma,k})^T
\]
\[
= (I_3 + hQ_{\sigma,k}) \left( \sum_{i \in I_\sigma} \theta_{i,k}^T \right) (I_3 + hQ_{\sigma,k})^T = (I_3 + hQ_{\sigma,k})\Sigma_{\sigma,k}(I_3 + hQ_{\sigma,k})
\]
which means that
\[
\delta \Sigma_k = \Sigma_{k+1} - \Sigma_k = hQ_{\sigma,k} \Sigma_{\sigma,k} + h\Sigma_{\sigma,k} Q_{\sigma,k} + h^2 Q_{\sigma,k} \Sigma_{\sigma,k} Q_{\sigma,k}
\].

Remark C.3. The term \( h^2 Q_{\sigma} \Sigma_{\sigma} Q_{\sigma} \) in Proposition C.2 corresponds to the term \( \delta g_1 \cdot \delta g_2 \) in the “product rule” for \( \delta \) (Lemma B.4 (c)). It vanishes when using negative gradient flow. In our case, it does not affect the qualitative behavior of gradient descent.

The following lemma shows relations between several quantities from Definition C.1.

Lemma C.4. Let \( M > 0 \). For \( \sigma \in \{\pm 1\} \) and \( x \in \mathbb{R} \), we have
\[
f_{W,\tau,\sigma}(x) = p_\sigma x + q_\sigma
\]
\[
\hat{u}_\sigma = -M_\sigma \hat{v}_\sigma
\].

Moreover,
\[
\hat{u} = B\hat{v}, \quad \hat{u} = -M\tilde{v}, \quad \tilde{v} = B\hat{v} + \begin{pmatrix} 0 \\ c \\ 0 \\ c \end{pmatrix}
\].
Proof. For \( x \in \mathbb{R} \),
\[
f_{W,\tau,\sigma}(x) = c + \sum_{i \in I} w_i \varphi'(\tau_i \sigma)(a_i x + b_i)
= c + \sum_{i \in I} (w_i a_i x + w_i b_i) + \alpha \sum_{i \in I - \sigma} (w_i a_i x + w_i b_i) = p_\sigma x + q_\sigma .
\]
Therefore, using Definition 7,
\[
\hat{u}_\sigma = \begin{pmatrix} \hat{r}_\sigma \\ \hat{s}_\sigma \end{pmatrix} = -\frac{1}{n} \left( \sum_{j \in J_\sigma} \left( f_{W,\tau,\sigma}(x_j) - y_j \right) x_j \right)
= -\frac{1}{n} \left( \sum_{j \in J_\sigma} \left( p_\sigma x_j + q_\sigma - y_j \right) x_j \right)
= -\frac{1}{n} \left( p_\sigma \sum_{j \in J_\sigma} x_j^2 + q_\sigma \sum_{j \in J_\sigma} x_j - \sum_{j \in J_\sigma} x_j y_j \right)
= -M_\sigma \left( p_\sigma \right) + \frac{1}{n} \sum_{j \in J_\sigma} \hat{u}^0_{\sigma j} = -M_\sigma \hat{u}_\sigma + \hat{u}^0_{\sigma} = -M_\sigma (v_\sigma - v_{\text{opt}}) = -M_\sigma v_\sigma .
\]
We now obtain
\[
\hat{u} = \begin{pmatrix} r_1 \\ s_1 \\ r_{-1} \\ s_{-1} \end{pmatrix} = \begin{pmatrix} \hat{r}_1 + \alpha \hat{r}_{-1} \\ \hat{s}_1 + \alpha \hat{s}_{-1} \\ \hat{r}_{-1} + \alpha \hat{r}_1 \\ \hat{s}_{-1} + \alpha \hat{s}_1 \end{pmatrix} = \tilde{B} \hat{u}
\]
\[
\tilde{u} = \begin{pmatrix} \hat{u}_1 \\ \hat{u}_{-1} \end{pmatrix} = \begin{pmatrix} M_1 \\ M_{-1} \end{pmatrix} \begin{pmatrix} \tilde{v}_1 \\ \tilde{v}_{-1} \end{pmatrix} = \tilde{M} \tilde{v}
\]
\[
\hat{v} = \begin{pmatrix} p_1 \\ q_1 \\ p_{-1} \\ q_{-1} \end{pmatrix} = \begin{pmatrix} \hat{p}_1 + \alpha \hat{p}_{-1} \\ \hat{q}_1 + \alpha \hat{q}_{-1} \\ \hat{p}_{-1} + \alpha \hat{p}_1 \\ \hat{q}_{-1} + \alpha \hat{q}_1 \end{pmatrix} = \tilde{B} \hat{v} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} .
\]
This enables us to compute another iteration equation:

**Proposition C.5.** Let \( M > 0 \). Then,
\[
\delta \tilde{v} = -h A \tilde{M} \tilde{v} = -h (\tilde{B}(G^w + \tilde{G}^{ab} + h \tilde{G}^{wab}) + \tilde{C}) \tilde{M} \tilde{v}
\]
\[
\delta \tilde{v} = -h A \tilde{M} \tilde{v} = -h (B(G^w + G^{ab} + h G^{wab}) + C) \tilde{M} \tilde{v} .
\]
Hence,
\[
\tilde{v}_{k+1} = \tilde{v}_k + \delta \tilde{v}_k = (I_4 - h A_k M) \tilde{v}_k .
\]

**Proof.** Consider
\[
\tilde{v}_\sigma = \begin{pmatrix} \tilde{p}_\sigma \\ \tilde{q}_\sigma \end{pmatrix} = \begin{pmatrix} \Sigma_{\sigma,wa} \\ \Sigma_{\sigma,wb} \end{pmatrix} = \begin{pmatrix} I_2 \\ 0 \end{pmatrix} \Sigma_\sigma \begin{pmatrix} 0 \\ 1 \end{pmatrix} .
\]
Using Proposition C.2 and Lemma B.4 we obtain
\[
\delta \tilde{v}_\sigma = \begin{pmatrix} I_2 \\ 0 \end{pmatrix} \begin{pmatrix} h Q_\sigma \Sigma_\sigma + h \Sigma_\sigma Q_\sigma + \hbar^2 Q_\sigma \Sigma_\sigma Q_\sigma \end{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \begin{pmatrix} \Sigma_{\sigma,wa}^2 \\ \Sigma_{\sigma,wb}^2 \end{pmatrix} \begin{pmatrix} r_\sigma \\ s_\sigma \end{pmatrix} = h \begin{pmatrix} 0 \\ 0 \\ r_\sigma \end{pmatrix} \begin{pmatrix} \Sigma_{\sigma,wa} \\ \Sigma_{\sigma,wb} \end{pmatrix} + h \begin{pmatrix} \Sigma_{\sigma,ab} \Sigma_{\sigma,wa} \\ \Sigma_{\sigma,wb} \Sigma_{\sigma,ab} \end{pmatrix} \begin{pmatrix} r_\sigma \\ s_\sigma \end{pmatrix} .
\]
While this system has a dimension independent of \( v \), we see that the systems for \( \Sigma \) have different dimensions. Since \( \tilde{v} \) is three-dimensional and \( \delta c \) is one-dimensional, we always have systems that are effectively three-dimensional, which reduces the dimension from 22 to 16. Moreover, we always have some redundancy among the parameters although its dimension does not depend on \( v \). However, removing these redundancies is not beneficial for our analysis.

Therefore, \( \delta \tilde{v} = h \left( \tilde{G}^w + \tilde{G}^{ab} + \tilde{h}G^{wab} \right) \tilde{u} \). Also,

\[
\delta \tilde{v} = \tilde{B} \delta \tilde{v} + \delta \begin{pmatrix} 0 \\ c \\ 0 \end{pmatrix} = \tilde{B} h \left( \tilde{G}^w + \tilde{G}^{ab} + \tilde{h}G^{wab} \right) \tilde{u} + h \tilde{C} \tilde{u}
\]

We can now use the identities from Lemma C.4 and the fact that \( \tilde{v} - \tilde{v} = \hat{v}^{\text{opt}} \) is constant to compute

\[
\delta \tilde{v} = \tilde{B} \delta \tilde{v} + \delta \begin{pmatrix} 0 \\ c \\ 0 \end{pmatrix} = \tilde{B} h \left( \tilde{G}^w + \tilde{G}^{ab} + \tilde{h}G^{wab} \right) \tilde{u} + h \tilde{C} \tilde{u}
\]

Since \( \tilde{P}^2 = I_4 \), it follows that

\[
\delta \tilde{v} = \delta (\tilde{P} \tilde{v}) = \tilde{P} \delta \tilde{v} = -h \tilde{P} \tilde{A} \tilde{M} \tilde{v} = -h \tilde{P} \tilde{A} \tilde{P} \tilde{P} \tilde{M} \tilde{P} \tilde{v} = -h \tilde{A} \tilde{M} \tilde{v}
\]

and

\[
A = \tilde{P} \tilde{A} \tilde{P} = \tilde{P} \left( \tilde{B} \tilde{P} \tilde{P} \tilde{G}^w + \tilde{G}^{ab} + \tilde{h}G^{wab} \right) \tilde{P} \tilde{B} + \tilde{C} \right) \tilde{P}
\]

\[
= B(G^w + G^{ab} + hG^{wab})B + C.
\]

**D Comments**

In this section, we provide some remarks on the interpretation of the gradient descent equations derived in Appendix C.

**Remark D.1 (System decomposition).** We have so far derived different “systems”, i.e. results on how quantities evolve during gradient descent. These systems and their dependencies are depicted in Figure D.1. In particular, we see that the systems for \( \Sigma_1, \Sigma_{-1} \) and \( \tilde{v} \) together yield a 22-dimensional system that does not depend on any other quantities. This 22-dimensional system describes some central properties of the neural network parameters \( W \) although its dimension does not depend on \( m \). These properties include:

- Slope \( p_\sigma \) and intercept \( q_\sigma \) for both signs \( \sigma \in \{\pm 1\} \).
- The loss \( L_{D,\tau}(W) \), which can be computed from \( p_\sigma \) and \( q_\sigma \).

While this system has a dimension independent of \( m \), the probability distribution over its initialization may well depend on \( m \). If its evolution is known, the evolution \( (W_k)_{k \in \mathbb{N}_0} \) can be determined by solving \( m \) independent three-dimensional systems and the one-dimensional system \( \delta c = h(\tilde{s}_1 + \tilde{s}_{-1}) \). Here, we will proceed along similar lines: We will first analyze the behavior of the 22-dimensional system and then apply our results to the three-dimensional systems.

In fact, the 22-dimensional system can be reduced to a 14-dimensional system: The matrices \( \Sigma_\sigma \) are always symmetric and thus effectively 6-dimensional, which reduces the dimension from 22 to 16. Moreover, we always have

\[
\begin{pmatrix} p_1 \\ p_{-1} \end{pmatrix} = \begin{pmatrix} 1 & \alpha \\ \alpha & 1 \end{pmatrix} \begin{pmatrix} \Sigma_{1,wa} \\ \Sigma_{-1,wa} \end{pmatrix}.
\]

However, removing these redundancies is not beneficial for our analysis.
Recall that the components of the equation $\delta v = -hAMv$ in Proposition C.5 can be interpreted as follows:

$$G^w_\sigma = \begin{pmatrix} \Sigma_{\sigma, w^2} & 0 \\ 0 & \Sigma_{\sigma, w^2} \end{pmatrix}, \quad G^{ab}_\sigma = \begin{pmatrix} \Sigma_{\sigma, a^2} & \Sigma_{\sigma, ab} \\ \Sigma_{\sigma, ab} & \Sigma_{\sigma, b^2} \end{pmatrix}, \quad G^{wab}_\sigma = (r_\sigma \Sigma_{\sigma, wa} + s_\sigma \Sigma_{\sigma, wb})I_2,$$

$$\hat{B} = \begin{pmatrix} I_2 \\ \alpha I_2 \end{pmatrix}, \quad \hat{C} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix},$$

$$\hat{A} = \hat{B} \left( G^w_1 + G^{ab}_1 + hG^{wab}_1 \right) \hat{B} + \hat{C}.$$

- The matrix $G^w_\sigma \succeq 0$ describes the improvement of $v_\sigma$ by updating the weights $(a_i)_{i \in I_\sigma}$ and $(b_i)_{i \in I_\sigma}$. The larger $|w_i|$, the larger the gradients $\frac{\partial L_{D, \tau}}{\partial w_i}$ and $\frac{\partial \tilde{L}_{D, \tau}}{\partial w_i}$ and the more effect does a change in $a_i, b_i$ have on the overall function $f_{W, \tau, \sigma}$.
- The matrix $G^{ab}_\sigma$ is also positive semidefinite since $\text{tr}(G^{ab}_\sigma) \geq 0$ and $\det(G^{ab}_\sigma) = \Sigma_{\sigma, a^2} \Sigma_{\sigma, b^2} - \Sigma_{\sigma, ab}^2 \geq 0$ due to Cauchy-Schwarz. It describes the improvement of $v_\sigma$ by updating the weights $(w_i)_{i \in I_\sigma}$. Larger values of $|a_i|, |b_i|$ mean stronger effects of changing $w_i$. If the vectors $(a_i)_{i \in I_\sigma}$ and $(b_i)_{i \in I_\sigma}$ are linearly dependent (perfectly correlated), e.g. at initialization because of $b_i, 0 = 0$, then $G^{ab}_\sigma$ only has rank one and changing the $w_i$ cannot independently update both components of $v_\sigma$. Recall that the components of $\tilde{v}_\sigma$ are the differences of the slope and intercept of $f_{W, \tau, \sigma}$ to the optimal linear regression slope and intercept, respectively.
- The matrix $\hat{B}$ causes an interaction between both signs $\sigma \in \{\pm 1\}$ if the leaky parameter $\alpha$ is nonzero. If it is zero, the hidden neurons are only active for one sign $\sigma$ and do only interact indirectly via the bias $c$.
- The matrix $\hat{C}$ describes the improvement of $v_\sigma$ by updating the bias $c$. It is not block-diagonal since $c$ is active for both signs $\sigma \in \{\pm 1\}$, however, $\hat{C}$ only has rank one since changing $c$ can only change $q_1$ and $q_{-1}$ by the same amount. $\hat{C}$ is positive semidefinite since it is symmetric and it has eigenvectors $e_1, e_3, (0, 1, 0, -1)$ to the eigenvalue 0 and $(0, 1, 0, 1)$ to the eigenvalue 2.
- The matrix $G^{wab}_\sigma$ represents parts of the error that (discrete) gradient descent makes when trying to approximate negative gradient flow. It arises from the additional term $\delta g_1 \cdot \delta g_2$ in the product rule for $\delta$ (Lemma B.4 (c)) and does not need to be positive semidefinite. If $h$ is too large, the matrix $\hat{A}$ might therefore not be positive semidefinite.
Remark D.3 (Discretization error). We have already seen that the systems for $\Sigma_0$ and $\overline{v}$ are affected by terms that arise from the term $\delta g_1 \cdot \delta g_2$ in the “discrete product rule” of Lemma B.4 (c). We will see that in our scenario (with small enough step size), these “disturbances” are small enough to not influence the qualitative behavior of gradient descent. There is also an invariant that holds when using negative gradient flow but breaks down when using gradient descent: In the former case, $a_1^2 + b_1^2 - w_1^2$ remains constant during the optimization for each $i \in I$. An analogous identity for linear networks has been observed by Saxe et al. [2014]. ▲

Remark D.4 (Alternative systems). In some special cases, the approach presented here only works if we modify the systems. For example, the assumption $M > 0$ is not satisfied if the dataset is contained in $(0, \infty)$ since this implies $M_{-1} = 0$. In this case, the system $\delta \overline{v} = -hA\overline{M}\overline{v}$ could be reduced to a two-dimensional system since $p_{-1}$ and $q_{-1}$ are irrelevant for the loss. We will also see that the argument here does not work for $|\alpha| = 1$ since this renders the matrix $B$ singular. The case $\alpha = 1$ corresponds to a linear activation function $\varphi(x) = x$, which implies $p_1 = p_{-1}$ and $q_1 = q_{-1}$. Similarly, the case $\alpha = -1$ corresponds to $\varphi(x) = |x|$, which implies $p_1 = -p_{-1}$. In both cases, the dimension of $v$ could be reduced. ▲

Figure D.2: Optimal affine regression lines for $D_1$ (orange, upper line) and $D_{-1}$ (blue, lower line) for an example dataset $D$. The data points are shown in black. The slope and intercept of the optimal affine regression line for $D_\sigma$ are given by $p_{D,\sigma}^{opt}$ and $q_{D,\sigma}^{opt}$, respectively.

Remark D.5 (Affine regression optimum). Here, we review some well-known properties of performing affine least-squares regression on a dataset $D$. This analysis also applies to $D_1$ and $D_{-1}$. Consider

$$X := \begin{pmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{pmatrix}, \quad y := \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad v := \begin{pmatrix} p \\ q \end{pmatrix}. $$

We always have $X^\top X \succeq 0$. Assume that $X$ has full column rank such that $X^\top X \succ 0$. The least-squares risk of an affine function $f_v(x) = px + q$ is $R_D(f_v)$ with

$$2nR_D(f_v) = \sum_{j=1}^n (y_j - f_v(x_j))^2 = \|y - Xv\|^2 = (y - Xv)^\top(y - Xv)$$

$$= \left(v - (X^\top X)^{-1}X^\top y\right)^\top X^\top X \left(v - (X^\top X)^{-1}X^\top y\right) + \left(y^\top y - y^\top X(X^\top X)^{-1}X^\top y\right), \quad (3)$$

where we performed a completion of the square. The optimal affine function has therefore parameters

$$v^{opt} = (X^\top X)^{-1}X^\top y = \left(\frac{1}{n} \sum_j x_j y_j \right)^{\frac{1}{2}} \left(\frac{1}{n} \sum_j x_j y_j \right)^{-1} \left(\frac{1}{n} \sum_j x_j y_j \right).$$

Note that applying Eq. [3] to $D_1$ and $D_{-1}$ after some rearrangement yields

$$L_{D,\tau}(W) = \frac{1}{2} (v - v^{opt}_D)^\top M_D (v - v^{opt}_D) + \text{const} = \frac{1}{2} \overline{v}^\top M_D \overline{v} + \text{const},$$

where the constant term is the optimal achievable loss by affine regression on $D_1$ and $D_{-1}$. ▲
E Stochastic Proofs

In this section, we show that $W_0$ and $D$ likely have certain properties. The results are formulated in Proposition E.3 and Proposition E.5, respectively. In order to obtain these results, we employ concentration inequalities. Besides Markov’s inequality, we use Hoeffding’s inequality:

**Lemma E.1** (Hoeffding’s inequality, e.g. Lemma A.3 in Györfi et al. [2002]). Let $(\Omega, \mathcal{F}, P)$ be a probability space, $a < b$, $n \geq 1$ and $X_1, \ldots, X_n : \Omega \to [a, b]$ be independent random variables. Then, for $\tau \geq 0$, we have

$$P \left( \frac{1}{n} \sum_{i=1}^{n} (X_i - \mathbb{E}X_i) \geq (b-a) \sqrt{\frac{\tau}{2n}} \right) \leq 2e^{-\tau}.$$ 

Using Markov and Hoeffding, we can prove an asymptotic concentration result. The intuition behind this result is that for random variables $X_1, \ldots, X_n$ with mean zero and finite variance, the value $n^{-1/2} (X_1 + \ldots + X_n)$ asymptotically has a Gaussian distribution by the central limit theorem. The tail of the Gaussian distribution decreases stronger than any inverse polynomial: If $\Phi$ is the CDF of a Gaussian distribution, then $\Phi(\beta n^{\varepsilon}) = O(n^{-\gamma})$ for all $\beta, \varepsilon, \gamma > 0$, where the constant in $O(n^{-\gamma})$ depends on $\beta, \varepsilon, \gamma$. However, the central limit theorem does not tell us how close the CDF of $n^{-1/2} (X_1 + \ldots + X_n)$ is to $\Phi$, so we use Markov’s and Hoeffding’s inequalities instead.

**Lemma E.2.** Let $Q$ be a probability distribution on $\mathbb{R}$ with $\mu_p := \int |x|^p dQ(x) < \infty$ for all $p \in (1, \infty)$. For $n \in \mathbb{N}$, let $(\Omega_n, \mathcal{F}_n, P_n)$ be probability spaces with independent $Q$-distributed random variables $X_{n1}, X_{n2}, \ldots, X_{nn} : \Omega_n \to \mathbb{R}$. Then, the random variables $S_n := \frac{1}{n} \sum_{i=1}^{n} X_{ni}$ satisfy

$$P_n \left( |S_n - \mathbb{E}S_n| \geq \beta n^{\varepsilon - 1/2} \right) = O(n^{-\gamma})$$

for all $\beta, \varepsilon, \gamma > 0$, where the constant in $O(n^{-\gamma})$ may depend on $\beta, \varepsilon, \gamma$ (cf. Definition A.2).

**Proof.** Let $\beta, \varepsilon, \gamma > 0$ be fixed. For $n \in \mathbb{N}$ and $b > 0$ to be determined later, define $B := \{\max_{1 \leq i \leq n} |X_{ni}| \leq b\}$. Then, for all $p > 0$,

$$P_n(B^c) \leq \sum_{i=1}^{n} P_n(|X_{ni}| \geq b) \leq n P_n(|X_{n1}|^p \geq b^p) \overset{\text{Markov}}{\leq} n \frac{\mathbb{E}P_n|X_{n1}|^p}{b^p} = n \frac{\mu_p}{b^p}.$$ 

(4)

Since $S_n = S_n \mathbb{1}B + S_n \mathbb{1}B^c$, we can now bound

$$P_n(|S_n - \mathbb{E}S_n| \geq \beta n^{\varepsilon - 1/2}) \leq \frac{1}{b} \sum_{i} P_n(|S_n \mathbb{1}B - \mathbb{E}(S_n \mathbb{1}B)| \geq \beta n^{\varepsilon - 1/2} / 2) + \frac{1}{b} P_n(|S_n \mathbb{1}B^c - \mathbb{E}(S_n \mathbb{1}B^c)| \geq \beta n^{\varepsilon - 1/2} / 2).$$

With $\tau := \gamma \log n$ and $b := \beta n^{\varepsilon} \sqrt{\frac{1}{8\gamma \log n}}$, we have

$$(b - (-b)) \sqrt{\frac{\tau}{2n}} = 2 \beta n^{\varepsilon} \sqrt{\frac{1}{8\gamma \log n}} \cdot \sqrt{\frac{\gamma \log n}{2n}} = \beta n^{\varepsilon - 1/2} / 2$$

and hence, Hoeffding (Lemma E.1) applied to $X_i := X_{ni} \mathbb{1}|X_{ni}| \leq b$ yields

$$I \leq 2e^{-\tau} = 2n^{-\gamma}.$$ 

Moreover, we have

$$\|\mathbb{E}P_n(S_n \mathbb{1}B^c)\| \leq \|S_n \mathbb{1}B^c\|_{L_1(P_n)} \overset{\text{Hölder}}{\leq} \|S_n\|_{L_2(P_n)} \|\mathbb{1}B^c\|_{L_2(P_n)}$$

$$\leq \left( \frac{1}{n} \sum_{i=1}^{n} \|X_{ni}\|_{L_2(P_n)} \right) \|\mathbb{1}B^c\|_{L_2(P_n)} = \sqrt{n} \sqrt{P_n(B^c)}$$

$$\leq \sqrt{n} \frac{\mu_p}{b^p} = \sqrt{\mu_p \frac{\mu_p}{b^p} (8\gamma \log n)^p / 4} n^{(1-\varepsilon)p/2}.$$
If we choose \( p \geq 2/\varepsilon \), we have \((1-\varepsilon p)/2 \leq -1/2 < \varepsilon -1/2 \) and hence \(|\mathbb{E}(S_n 1_{B^c})| < \beta n^{\varepsilon-1/2}/2 \) for \( n \) large enough. Now, let \( n \) be sufficiently large. For \( \omega \in B \), we have \( S_n(\omega) 1_{B^c}(\omega) = 0 \) and hence \(|S_n(\omega) 1_{B^c}(\omega) - \mathbb{E}(S_n 1_{B^c})| < \beta n^{\varepsilon-1/2}/2 \). Thus,

\[
II \leq P(B^c) \leq n \frac{\mu_p}{\beta^p} = \frac{\mu_p}{\beta^p} \cdot (8\gamma \log n)^p/2 n^{1-\varepsilon p} .
\]

If we choose \( p > (1+\gamma)/\varepsilon \), then \( 1-\varepsilon p < -\gamma \) and hence II = \( O(n^{-\gamma}) \).

Now, we can prove that certain properties of the initialization \( W_0 \) hold with high probability. We will see that in all properties except (W4), the tails of the probability distributions decrease so quickly that only the parameter \( \gamma \) in (W4) is relevant for the rate of convergence.

**Proposition E.3.** Let \( \varepsilon, \gamma > 0 \) and let \( W_0 \) be distributed as in Assumption 2. Then, the properties

(W1) \( b_{i,0} = c_0 = 0 \),
(W2) \( \max_i |w_{i,0}| \leq m^{-1/2+\varepsilon} \),
(W3) \( \max_i |a_{i,0}| \leq m^\varepsilon \),
(W4) \( \min_i |a_{i,0}| \geq m^{-(1+\gamma)} \),
(W5) \( \Sigma_{\sigma,a} = \frac{1}{4} \left(m \text{Var}(Z_{\sigma})\right) \text{Var}(Z_a) \) for all \( \sigma \in \{\pm 1\} \),
(W6) \( \Sigma_{\sigma,w,a} = \frac{1}{4} \left(\text{Var}(Z_{\sigma})\right) \text{Var}(Z_{wa}) \) for all \( \sigma \in \{\pm 1\} \),
(W7) \( \|\epsilon\|_{\infty} \leq m^\varepsilon \) for all \( \epsilon \in \{\pm 1\} \).

are satisfied with probability \( \geq 1 - O(m^{-\gamma}) \), where the constant in \( O(m^{-\gamma}) \) may depend on \( \varepsilon \) and \( \gamma \) (cf. Definition A.3).

**Proof.** We will show the statement for each of the properties (W1) – (W7) individually, the rest follows by the union bound. Let \( Z_a, Z_w \) be the random variables from Assumption 2.

By property (Q2) in Assumption 2, \( \mathbb{E}|Z_a|^p, \mathbb{E}|Z_w|^p < \infty \) for all \( p \in (0, \infty) \). It can be shown (using the Minkowski and Hölder inequalities) that all other random variables used below satisfy the same property, which we will use in order to apply Lemma E.2.

(W1) True by Assumption 2.

(W2) By the Markov inequality, for \( p > 0 \),

\[
P_m^{\text{init}} \left( |w_{i,0}| \geq m^{-1/2+\varepsilon} \right) = P_m^{\text{init}} \left( |w_{i,0}|^p \geq m^{-(1-1/2+\varepsilon)p} \right) \leq \frac{\mathbb{E}|w_{i,0}|^p}{m^{-(1/2+\varepsilon)p}} \leq \frac{\mathbb{E}|Z_w|^p}{m^{-(1/2+\varepsilon)p}} = \mathbb{E}(|Z_w|^p)m^{-\varepsilon p} .
\]

By choosing \( p = (1+\gamma)/\varepsilon \), we can use the union bound to conclude

\[
P_m^{\text{init}} \left( \max_i |w_{i,0}| \geq m^{-1/2+\varepsilon} \right) \leq m \cdot \mathbb{E}(|Z_w|^p)m^{-\varepsilon p} = O(m^{-\varepsilon p}) = O(m^{-\gamma}) .
\]

(W3) Similar to (W2).

(W4) By property (Q1) of Assumption 2, \( Z_a \) has a probability density \( p_a \) that is bounded by \( B_Z^{wa} \). Thus, for all \( \delta \geq 0 \), we obtain

\[
P_m^{\text{init}}(\{a_{i,0} \leq \delta\}) = P(|Z_a| \leq \delta) = \int_{-\delta}^\delta p_a(x) \, dx \leq 2\delta \cdot B_Z^{wa} .
\]

Therefore,

\[
P_m^{\text{init}} \left( \min_i |a_{i,0}| \leq m^{-(1+\gamma)} \right) \leq \sum_{i=1}^m P_m^{\text{init}}(\{a_{i,0} \leq m^{-(1+\gamma)}\}) \leq m \cdot 2m^{-(1+\gamma)} \cdot B_Z^{wa} = O(m^{-\gamma}) .
\]

(W5) For the next three properties, we need some preparation. Let

\[
A_{\sigma,i} := 1_{(0,\infty)}(\sigma a_{i,0})a_{i,0}
\]
\[ W_{\sigma,i} := \mathbb{I}_{(0,\infty)}(\sigma a_{i,0}) w_{i,0} . \]

Note that the indicator function is applied to \( \sigma a_{i,0} \) in both definitions. Then, \( \Sigma_{\sigma,a^2,0} = \sum_{i \in I_m} a_{i,0}^2 = \sum_{i=1}^m A_{\sigma,i}^2 \) and similarly for \( \Sigma_{\sigma,w^2,0} \) and \( \Sigma_{\sigma,wa,0} \). We obtain

\[
\mathbb{E}_{P_m} A_{\sigma,i}^2 = \int A_{\sigma,i}^2 \, dP_m^{\text{init}} = \int (\mathbb{I}_{(0,\infty)}(\sigma a_{i,0}))^2 \, dP_m^{\text{init}} = \int (\sigma a_{i,0} > 0) a_{i,0}^2 \, dP_m^{\text{init}}.
\]

\[
= \int_{(0,\infty)} x^2 p_a(x) \, dx \overset{(Q1)}{=} \frac{1}{2} \int_{\mathbb{R}} x^2 p_a(x) \, dx = \frac{\mathbb{E}(Z_a^2)}{2} \overset{(Q1)}{=} \frac{\text{Var}(Z_a)}{2} .
\]

\[
\mathbb{E}_{P_m} W_{\sigma,i}^2 = \mathbb{E}_{P_m} \left( (\mathbb{I}_{(0,\infty)}(\sigma a_{i,0}))^2 w_{i,0}^2 \right) \overset{\text{indep.}}{=} \left( \mathbb{E}_{P_m} \left( \mathbb{I}_{(0,\infty)}(\sigma a_{i,0}) \right)^2 \right) \cdot \left( \mathbb{E}_{P_m} w_{i,0}^2 \right).
\]

\[
= P_m^{\text{init}}(\sigma a_{i,0} > 0) \cdot \mathbb{E} \left( m^{-1/2} Z_w \right)^2 \overset{(Q1)}{=} \frac{1}{2} \cdot \frac{\text{Var}(Z_w)}{m} .
\]

\[
\mathbb{E}_{P_m} W_{\sigma,i} A_{\sigma,i} = \mathbb{E}_{P_m} \left( \mathbb{I}_{(0,\infty)}(\sigma a_{i,0}) w_{i,0} a_{i,0} \right) \overset{\text{indep.}}{=} \left( \mathbb{E}_{P_m} w_{i,0} \right) \cdot \left( \mathbb{E}_{P_m} \mathbb{I}_{(0,\infty)}(\sigma a_{i,0}) a_{i,0} \right) = 0 .
\]

Now, define

\[
S_m := \frac{\Sigma_{\sigma,a^2,0}}{m} = \frac{1}{m} \sum_{i=1}^m A_{\sigma,i}^2 ,
\]

which is an average of \( m \) i.i.d. variables that are \( p \)-integrable for every \( p > 0 \). Then, \( \mathbb{E}_{P_m} S_m = \mathbb{E}_{P_m} A_{\sigma,1}^2 = \text{Var}(Z_a)/2 \) and with \( \epsilon = 1/2, \beta = \text{Var}(Z_a)/4 \) yields:

\[
P_m^{\text{init}} \left( \left| S_m - \frac{\text{Var}(Z_a)}{2} \right| \geq \frac{\text{Var}(Z_a)}{4} \right) \leq O(m^{-\gamma \rho}) .
\]

Hence,

\[
P_m^{\text{init}}(\Sigma_{\sigma,a^2,0} \notin [m \text{Var}(Z_a)/4, m \text{Var}(Z_a)]) = P_m^{\text{init}}(S_m \notin [\text{Var}(Z_a)/4, \text{Var}(Z_a)]) \leq P_m^{\text{init}}(S_m \notin [\text{Var}(Z_a)/4, 3 \text{Var}(Z_a)/4]) \leq O(m^{-\gamma \rho}) .
\]

(W6) An analogous argument yields \( P_m^{\text{init}}(\Sigma_{\sigma,w^2,0} \notin [\text{Var}(Z_w)/4, \text{Var}(Z_w)]) \leq O(m^{-\gamma \rho}) .
\]

(W7) Let \( S_m := \frac{1}{m} \sum_{i=1}^m A_{\sigma,i} \cdot \sqrt{m} W_{\sigma,i} = \Sigma_{\sigma,wa,0}/\sqrt{m} . \) Then, \( \mathbb{E}_{P_m} S_m = 0 \) and thus

\[
P_m^{\text{init}}(\Sigma_{\sigma,wa,0} \geq m^\epsilon) = P_m^{\text{init}}(\left| S_m \right| \geq m^{\epsilon-1/2}) \leq O(m^{-\gamma \rho}) .
\]

Now, we want to investigate stochastic properties of the dataset. In order to show that \( M_D^{-1} \) is likely close to \( M_{\text{data}}^{-1} \) (both are defined in Definition 7), we need the following lemma, which is similar for example to Theorem 2.3.4 in [1989].

**Lemma E.4.** Let \( A, B \in \mathbb{R}^{m \times m} \) and let \( \| \cdot \| \) be a matrix norm on \( \mathbb{R}^{m \times m} \). If \( A \) is invertible and \( \| A^{-1} \| \| A - B \| < 1 \), then \( B \) is invertible with

\[
\| B^{-1} - A^{-1} \| \leq \| A^{-1} \| \| A - B \| \| B^{-1} \| , \quad \| B^{-1} \| \leq \frac{\| A^{-1} \|}{1 - \| A^{-1} \| \| A - B \|} .
\]

**Proof.** We have \( B = A(I - A^{-1}(A - B)) \) and since \( \| A^{-1}(A - B) \| \leq \| A^{-1} \| \| A - B \| < 1 \), the Neumann series implies that

\[
(I - A^{-1}(A - B))^{-1} = \sum_{k=0}^\infty (A^{-1}(A - B))^k .
\]

Hence \( B \) is invertible with \( B^{-1} - A^{-1} = A^{-1}(A - B)B^{-1} \) and

\[
B^{-1} = (I - A^{-1}(A - B))^{-1} A^{-1} = \sum_{k=0}^\infty (A^{-1}(A - B))^k A^{-1} ,
\]

which yields both bounds using the submultiplicativity of \( \| \cdot \| . \)

□
Now, we can show that for large $n$, a sampled dataset $D$ likely has characteristics that are close to $P^\text{data}$. We use the convention $\infty \cdot 0 := \infty$.

**Proposition E.5.** Let $P^\text{data}$ satisfy Assumption 13. Let $\varepsilon, K_{\text{data}} > 0$, $m \geq 1$ and $\gamma, \gamma' \geq 0$. If $\eta = \infty$, we further assume that $K_{\text{data}}$ satisfies $P^\text{data}((-K_{\text{data}}, K_{\text{data}}) \times \mathbb{R}) = 0$. Finally, let $D$ be a dataset with $n$ data points $(x_j, y_j)$ sampled independently from $P^\text{data}$. Then with probability $1 - O(n^{-\gamma} + nm^{-\eta\gamma})$ the following hold:

(D1) \[ \|v_D^\text{opt} - v_P^\text{opt}\|_\infty \leq n^{\varepsilon-1/2}, \]

(D2) For $\sigma \in \{\pm 1\}$, \[ \frac{1}{2}\lambda_{\min}(M_{\text{data}, \sigma}) \leq \lambda_{\min}(M_{D, \sigma}) \quad \text{and} \quad \lambda_{\max}(M_{D, \sigma}) \leq 2\lambda_{\max}(M_{\text{data}, \sigma}), \]

(D3) \[ \lambda_{\text{opt}} D \geq K_{\text{data}}n^{-\gamma}. \]

**Proof.** We use the shorthand $P := P^\text{data}$. Again, we bound the probabilities for each property separately.

(D1) For $\sigma \in \{\pm 1\}$, define

\[ S_n := (M_{D, \sigma})_{11} = \frac{1}{n} \sum_{j=1}^{n} I_{(0,\infty)}(\sigma x_j) x_j^2. \]

Then,

\[ \mathbb{E}_{P^n} S_n = \frac{1}{n} \sum_{j=1}^{n} \mathbb{E}_{D \sim P^n} \left( I_{(0,\infty)}(\sigma x_j) x_j^2 \right) = \mathbb{E}_{(x,y) \sim P} \left( I_{(0,\infty)}(\sigma x) x^2 \right) = (M_{P, \sigma})_{11}. \]

Because $P$ is bounded, it has finite moments and we can apply Lemma E.2. For all $\beta > 0$,

\[ P^n \left( |(M_{D, \sigma})_{11} - (M_{P, \sigma})_{11}| \geq \beta n^{(\varepsilon-1)/2} \right) = O(n^{-\gamma}). \]

We can get similar bounds for other entries of $M_{D, \sigma}$ and $\hat{u}_{D, \sigma}^0$. Since

\[ M_D - M_P = P \left( \begin{smallmatrix} M_{D,1} - M_{P,1} & 0 \\ 0 & M_{D,-1} - M_{P,-1} \end{smallmatrix} \right) \tilde{P}, \quad \hat{u}_D^0 = \tilde{P} \left( \begin{smallmatrix} 0 \\ \hat{u}_{D,-1}^0 \end{smallmatrix} \right), \]

and $\|\tilde{P}\| = 1$, the union bound implies that the following properties hold with probability $1 - O(n^{-\gamma'})$:

\[ |M_{D,\pm 1} - M_{P,\pm 1}| \leq 2\beta n^{(\varepsilon-1)/2}, \quad |M_D - M_P| \leq 2\beta n^{(\varepsilon-1)/2}, \quad \|\hat{u}_D^0 - \hat{u}_P^0\| \leq \beta n^{(\varepsilon-1)/2}. \quad (5) \]

Now assume that (5) holds. Set $A := M_P, B := M_D, a := \hat{u}_P^0, b := \hat{u}_D^0$. By condition (P1), $A$ is invertible. Without loss of generality, we can assume $\varepsilon < 1/2$. Then, for $n$ large enough,

\[ \|A^{-1}\|_\infty \|A - B\|_\infty \leq \|A^{-1}\|_\infty 2\beta n^{(\varepsilon-1)/2} \leq \frac{1}{2}. \]

Hence, Lemma E.4 implies that $B = M_D$ is invertible with $\|B^{-1}\|_\infty \leq 2\|A^{-1}\|_\infty$ and

\[ \|v_D^\text{opt} - v_P^\text{opt}\|_\infty = \|B^{-1}b - A^{-1}a\|_\infty \leq \|B^{-1}\|_\infty \|b - a\|_\infty + \|B^{-1} - A^{-1}\|_\infty \|a\|_\infty \leq \|B^{-1}\|_\infty (\|b - a\|_\infty + \|A^{-1}\|_\infty \|a\|_\infty \|B - A\|_\infty) \leq 4\|A^{-1}\|_\infty (1 + \|A^{-1}\|_\infty \|a\|_\infty) \beta n^{(\varepsilon-1)/2}. \]

We can choose $\beta > 0$ such that $4\|A^{-1}\|_\infty (1 + \|A^{-1}\|_\infty \|a\|_\infty) \beta \leq 1$. Therefore,

\[ \|v_D^\text{opt} - v_P^\text{opt}\|_\infty \leq n^{(\varepsilon-1)/2} \]

with probability $1 - O(n^{-\gamma'})$. 

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(D2) For $\sigma \in \{\pm 1\}$ and each $v \in \mathbb{R}^2$, we have
\[
|v^\top M_{D,\sigma} v - v^\top M_{P,\sigma} v| \leq \|v\|_2 \|M_{D,\sigma} - M_{P,\sigma}\|_2 \|v\|_2 \leq \sqrt{2}\|M_{D,\sigma} - M_{P,\sigma}\|_\infty \|v\|_2^2
\]
since $\|\cdot\|_2 \leq \sqrt{2}\|\cdot\|_\infty$ on $\mathbb{R}^{2 \times 2}$ as mentioned in Definition A.3. If we choose $\beta > 0$ small enough such that \(\frac{\beta}{\|M_{D,\sigma} - M_{P,\sigma}\|_\infty} \leq \min\{\lambda_\text{min}(M_{P,\sigma})/2, 1\}$, it follows that
\[
\lambda_\text{min}(M_{D,\sigma}) = \inf_{\|v\|_2 = 1} v^\top M_{D,\sigma} v \geq \inf_{\|v\|_2 = 1} v^\top M_{P,\sigma} v - |v^\top M_{P,\sigma} v - v^\top M_{D,\sigma} v| \\
\geq \lambda_\text{min}(M_{P,\sigma}) - \sqrt{2}\|M_{D,\sigma} - M_{P,\sigma}\|_\infty \geq \lambda_\text{min}(M_{P,\sigma})/2.
\]
Since (5) holds with probability $1 - O(n^{-\gamma})$, we have $\lambda_\text{min}(M_{D,\sigma}) \geq \lambda_\text{min}(M_{P,\sigma})/2$ with probability $1 - O(n^{-\gamma})$. The probability for $\lambda_\text{max}(M_{D,\sigma}) \leq 2\lambda_\text{max}(M_{P,\sigma})$ can be bounded similarly.

(D3) In the case $\eta = \infty$ and $P_X((-K_{\text{data}}, K_{\text{data}})) = 0$, this obviously holds with probability one since $K_{\text{data}}m^{-\gamma_{\text{data}}} \leq K_{\text{data}} \leq 2D$ almost surely. Otherwise, using property (P2) from Assumption 13 and the union bound yields
\[
P^n(\|x_D\| < K_{\text{data}}m^{-\gamma_{\text{data}}}) \leq \sum_{j=1}^{n} P^n(|x_j| < K_{\text{data}}m^{-\gamma_{\text{data}}}) \leq n \cdot O((K_{\text{data}}m^{-\gamma_{\text{data}}})^\eta) = O(nm^{-\eta\gamma_{\text{data}}}).
\]

\[\Box\]

#### F Reference Dynamics

In this section, we define a matrix $A^\text{ref} \approx A_0$ and study the asymptotic behavior of $h \sum_{k=0}^{\infty} \|\bar{v}_k\|$ when $\bar{v}_k$ satisfies a reference system
\[
\bar{v}_{k+1} = \bar{v}_k - h A^\text{ref} M_D \bar{v}_k,
\]
instead of the actual dynamics $\bar{v}_{k+1} = \bar{v}_k - h A_k M_D \bar{v}_k$. The solution of the reference system is simply $\bar{v}_k = (I - h A^\text{ref} M_D)^k \bar{v}_0$.

**Definition F.1.** Let $A^\text{ref} := B(G_0^{\text{w}} + G_0^{\text{ab}})B + C$, where $B, G^{\text{w}}, G^{\text{ab}}, C$ are defined in Definition C.1. Moreover, define the symmetric matrix
\[
H := M_D^{1/2} A^\text{ref} M_D^{1/2} = M_D^{1/2} (A^\text{ref} M_D) M_D^{-1/2}.
\]

**Assumption F.2.** Assume that $\gamma_{\psi}, \gamma_{\text{data}}, \gamma_{P} \geq 0$ with $\gamma_{\psi} + \gamma_{\text{data}} + \gamma_{P} < 1/2$. Moreover, we only consider initial vectors $W_0$ which satisfy the conditions (W1) – (W7) in Proposition E.3. Similar to Theorem 8, we further assume that
\[
K_{M}^{-1} \leq \lambda_\text{min}(M_D) \leq \lambda_\text{max}(M_D) \leq K_{M} \\
\psi_{D,P} = O(1) \\
\psi_{D,q} = O(m^{\gamma_{\psi} - 1}) \\
h \leq \lambda_\text{max}(H)^{-1} \\
0 < \varepsilon < \frac{1/2 - (\gamma_{\psi} + \gamma_{\text{data}} + \gamma_{P})}{3},
\]
where $K_M > 0$ is a constant and $H$ depends on $D$ and $W_0$. Note that since $\text{eig}(M_D) = \text{eig}(M_{D,1}) \cup \text{eig}(M_{D,-1})$, by construction of $M_D$, the first condition is equivalent to
\[
K_{M}^{-1} \leq \lambda_\text{min}(M_{D,\sigma}) \leq \lambda_\text{max}(M_{D,\sigma}) \leq K_{M} \text{ for } \sigma = \pm 1.
\]

**Lemma F.3.** Let Assumption F.2 be satisfied. The matrix $A^\text{ref}$ is of the form
\[
A^\text{ref} = \begin{pmatrix} A_1^\text{ref} & 0 \\ 0 & A_2^\text{ref} \end{pmatrix}
\]
with $0 < A_1^\text{ref}, A_2^\text{ref} \in \mathbb{R}^{2 \times 2}$ and
\[
\lambda_\text{min}(A_1^\text{ref}) = \Theta(m), \quad \lambda_\text{max}(A_1^\text{ref}) = \Theta(m), \quad \lambda_\text{min}(A_2^\text{ref}) = \Theta(1), \quad \lambda_\text{max}(A_2^\text{ref}) = \Theta(1).
\]
Proof. Since \( b_{t,0} = 0 \) by initialization property (W1) in Proposition E.3, we have \( \Sigma_{\sigma,ab,0} = \Sigma_{\sigma,b^2,0} = 0 \). Since the distributions of \( Z_a, Z_w \) have densities by (Q1) in Assumption 2, we have \( \text{Var}(Z_a), \text{Var}(Z_w) > 0 \). This yields

\[
G_{\sigma,0}^w + G_{\sigma,0}^{ab} = \left( \Sigma_{\sigma, a^2,0} + \Sigma_{\sigma, a^2,0} \right) \left( \begin{array}{c} \Theta(m) \\ \Theta(1) \end{array} \right).
\]

Hence,

\[
G_{0}^w + G_{0}^{ab} = \hat{P} \left( G_{0}^w + G_{0}^{ab} \right) \hat{P} = \hat{P} \left( G_{1,0}^w + G_{1,0}^{ab} \right) \hat{P} = \hat{P} \left( \begin{array}{c} \Theta(m) \\ \Theta(1) \end{array} \right) \hat{P} = \left( \begin{array}{c} \Theta(m) \\ \Theta(1) \end{array} \right) = (G_1, G_2).
\]

We have seen in Definition C.1 that

\[
B = \begin{pmatrix} \hat{B} \\ \hat{B} \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} 1 & \alpha \\ \alpha & 1 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} = (0, C).
\]

Using the previous results, we obtain

\[
A_{\text{ref}} = \begin{pmatrix} \hat{B} G_1 \hat{B} \\ \hat{B} G_2 \hat{B} + \hat{C} \end{pmatrix} = \begin{pmatrix} A_{\text{ref}}^1 \\ A_{\text{ref}}^2 \end{pmatrix}.
\]

The matrix \( \hat{B} \) is fixed and invertible since \( |\alpha| \neq 1 \). Moreover, \( \text{eig}(C) = \{0, 2\} \). This yields

\[
\text{eig}(A_{\text{ref}}^1) = \text{eig}(BG_1B) = \Theta(m), \quad \text{eig}(A_{\text{ref}}^2) = \text{eig}(BG_2B + C) = \Theta(1).
\]

\[\square\]

Proposition F.4. Let Assumption F.2 be satisfied. We have

\[
h \sum_{k=0}^{\infty} \| (I_4 - h A_{\text{ref}} M)^k v_0 \|_{\infty} = O(m^\varepsilon + \gamma^\psi - 1)
\]

\[
h \sum_{k=0}^{\infty} \| (I_4 - h A_{\text{ref}} M)^k \|_{\infty} = O(1).
\]

Proof. We divide the proof in multiple steps:

1. Investigate the initial vector:
   By definition, we have \( v_0 = v_0 - v_{\text{opt}}^D \). Therefore,

   \[
   |v_0| \leq |v_0| + |v_{\text{opt}}^D| \leq \begin{pmatrix} |p_{1,0}| \\ |p_{-1,0}| \\ |q_{1,0}| \\ |q_{-1,0}| \end{pmatrix} + \begin{pmatrix} \psi_{D,p} \\ \psi_{D,p} \\ \psi_{D,q} \\ \psi_{D,q} \end{pmatrix} = \begin{pmatrix} \Omega_0(m^\varepsilon) \\ \Omega_1(m^\varepsilon) \\ \Omega(m^\varepsilon) \\ \Omega(m^\varepsilon) \end{pmatrix} 
\]

   \[\text{Assumption F.2}, \text{(W7)}\]

   \[
   \sum_{k=0}^{\infty} \begin{pmatrix} O(m^\varepsilon) \\ O(m^\varepsilon) \\ O(1) \\ O(1) \end{pmatrix} \leq \begin{pmatrix} O(m^\varepsilon) \\ O(m^\varepsilon) \\ O(m^\varepsilon) \\ O(m^\varepsilon) \end{pmatrix} \leq \begin{pmatrix} O(m^\varepsilon) \\ O(m^\varepsilon) \end{pmatrix}.
\]

   Thus, we can group

   \[
   v_0 = \begin{pmatrix} v_{0,1} \\ v_{0,2} \end{pmatrix}
\]

   with \( v_{0,1}, v_{0,2} \in \mathbb{R}^2 \) and \( |v_{0,1}| = O(m^\varepsilon), |v_{0,2}| = O(m^\varepsilon) \).
(2) **Diagonalization yields a simple bound:**

The matrix $A^\text{ref}M$ is similar to the symmetric matrix

$$
H := M^{1/2} A^\text{ref} M^{1/2} = M^{1/2} (A^\text{ref} M) M^{-1/2} > 0.
$$

The matrix $H$ can thus be orthogonally diagonalized as $H = U D U^\top$ with $U$ orthogonal and $D$ diagonal such that $D$ contains the eigenvalues of $H$ in descending order. Then, $I_4 - hD$ only contains non-negative entries due to the condition $h \leq \lambda_{\max}(H)^{-1}$ with its maximal entry being $1 - h \lambda_{\min}(H)$. Thus, $\| (I_4 - hD)^k \|_2 = (1 - h \lambda_{\min}(H))^k$. By applying $(I_4 - hA^\text{ref} M)M^{-1/2} = M^{-1/2} - hA^\text{ref} M^{-1/2} = M^{-1/2}(I_4 - hH)^k$ inductively, we find $(I_4 - hA^\text{ref} M)^k M^{-1/2} = M^{-1/2}(I_4 - hH)^k$. We can now compute

$$
h \sum_{k=0}^{\infty} \| (I_4 - hA^\text{ref} M)^k \|_2 = h \sum_{k=0}^{\infty} \| M^{-1/2}(I_4 - hH)^k M^{1/2} \|_2
$$

$$
= h \sum_{k=0}^{\infty} \| M^{-1/2} U(I_4 - hD)^k U^\top M^{1/2} \|_2
$$

$$
\leq \| M^{-1/2} \|_2 \| M^{1/2} \|_2 \cdot h \sum_{k=0}^{\infty} \| (I_4 - hD)^k \|_2
$$

$$
= \text{cond}(M^{1/2}) h \sum_{k=0}^{\infty} (1 - h \lambda_{\min}(H))^k
$$

$$
= \frac{\text{cond}(M)}{\lambda_{\min}(H)} \leq O(1),
$$

where $\lambda_{\min}(H) \geq \Omega(1)$ since for $v \in \mathbb{R}^4$, we have

$$
v^\top H v = (M^{1/2} v)^\top A^\text{ref}(M^{1/2} v) \geq \lambda_{\min}(A^\text{ref}) v^\top M v \geq \lambda_{\min}(A^\text{ref}) \lambda_{\min}(M) v^\top v,
$$

where $\lambda_{\min}(A^\text{ref}) \lambda_{\min}(M) = \Theta(1)$ by Assumption F.2 and Lemma F.3.

(3) **AM has 2 “large” eigenvalues:**

Let

$$
M = \begin{pmatrix} M_{11} & M_{12} \\ M_{12}^\top & M_{22} \end{pmatrix}, \quad M^{1/2} = \begin{pmatrix} \tilde{M}_{11} & \tilde{M}_{12} \\ \tilde{M}_{12}^\top & \tilde{M}_{22} \end{pmatrix}
$$

be the block decompositions of $M$ and $M^{1/2}$ into $2 \times 2$ blocks. Then,

$$
M^{1/2} A^\text{ref} M^{1/2} = \begin{pmatrix} \tilde{M}_{11} A^\text{ref}_{11} \tilde{M}_{11} + \tilde{M}_{12} A^\text{ref}_{12} \tilde{M}_{12}^\top & * \\ * & * \end{pmatrix}
$$

and by Cauchy’s interlacing theorem (cf. e.g. Corollary III.1.5 in [Bhatia 2013]), the second largest eigenvalue $\lambda_2(H)$ of $H$ satisfies

$$
\lambda_2(H) \geq \lambda_2(\tilde{M}_{11} A^\text{ref}_{11} \tilde{M}_{11} + \tilde{M}_{12} A^\text{ref}_{12} \tilde{M}_{12}^\top) = \lambda_{\min}(\tilde{M}_{11} A^\text{ref}_{11} \tilde{M}_{11} + \tilde{M}_{12} A^\text{ref}_{12} \tilde{M}_{12}^\top)
$$

$$
\geq \lambda_{\min}(\tilde{M}_{11} A^\text{ref}_{11} \tilde{M}_{11}) \geq \lambda_{\min}(A^\text{ref}_{11}) \lambda_{\min}(M_{11})^2 \geq \lambda_{\min}(A^\text{ref}_{11}) \lambda_{\min}(M_{1/2})^2 = \lambda_{\min}(A^\text{ref}_{11}) \lambda_{\min}(M)
$$

$$
\geq \Theta(m).
$$

(4) **Lower components of eigenvectors to large eigenvalues are small:**

Let $w = (w_1, w_2)^\top$ be an eigenvector of $A^\text{ref} M$ with eigenvalue $\lambda \geq \lambda_2(H) \geq \Theta(m)$. The lower part of the identity $\lambda w = A^\text{ref} Mw$ reads as

$$
\lambda w_2 = A^\text{ref}_{22} M_{22} w_1 + A^\text{ref}_{22} M_{22} w_2,
$$

which yields

$$
\Theta(m) \| w_2 \|_2 \leq \lambda \| w_2 \|_2 \leq \| A^\text{ref}_{22} \|_2 \| M_{22} \|_2 \| w_1 \|_2 + \| A^\text{ref}_{22} \|_2 \| M_{22} \|_2 \| w_2 \|_2
$$

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\[ \leq \Theta(1)\|w_1\|_2 + \Theta(1)\|w_2\|_2 \]

and hence (for large \( m \))
\[ \|w_2\|_2 \leq \Theta(1) \frac{\Theta(1)}{\Theta(m) - \Theta(1)} \|w_1\|_2 = O(m^{-1})\|w_1\|_2 \]  
(9)

(5) The first two eigenvectors of \( A^\text{ref}M \) are “well-conditioned”:
Let
\[ U = \begin{pmatrix} U_1 & U_2 \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}, \quad F = \begin{pmatrix} F_1 & F_2 \end{pmatrix} := U_1^\top M^{1/2}, \quad W = \begin{pmatrix} W_1 \\ W_2 \end{pmatrix} := M^{-1/2}U_1. \]

The columns of \( W \) are the eigenvectors of \( A^\text{ref}M \) to the 2 largest eigenvalues:
\[ A^\text{ref}MW = M^{-1/2}M^{1/2}A^\text{ref}M^{1/2}U_1 = M^{-1/2}UDU^\top U_1 = M^{-1/2}UD \begin{pmatrix} I_2 \\ 0 \end{pmatrix} = M^{-1/2}U_1D_1 = WD_1, \]
where \( D_1 \) is the upper left 2 \( \times \) 2 block of \( D \). Thus,
\[ \|F\|_2 \leq \|U_1\|_2\|M^{1/2}\|_2 = 1 \cdot \lambda_{\max}(M^{1/2}) = \Theta(1) \]
\[ \|W\|_2 \leq \|M^{-1/2}\|\|U_1\|_2 = \lambda_{\max}(M^{-1/2}) \cdot 1 = \Theta(1) \]
\[ \|W_2\|_2 \leq \|W_2\|_F \leq O(m^{-1})\|W_1\|_F \leq O(m^{-1})\|W_2\|_2 \leq O(m^{-1}). \]

We want to show that \( W_1^{-1} \) exists and \( \|W_1^{-1}\|_2 \) is sufficiently small. Observe that \( I_2 = U_1^\top U_1 = FW = F_1W_1 + F_2W_2 \) and
\[ \|F_2W_2\|_2 \leq \|F_2\|_2\|W_2\|_2 \leq O(m^{-1}) \leq \frac{1}{2} \]
for large \( m \). Hence, \( F_1W_1 = I_2 - F_2W_2 \) is invertible with
\[ (F_1W_1)^{-1} = \sum_{k=0}^{\infty} (F_2W_2)^k, \quad \|(F_1W_1)^{-1}\|_2 \leq \sum_{k=0}^{\infty} \|F_2W_2\|_2^k \leq 2. \]

Since \( F_1W_1 \) has full rank, \( W_1 \) and \( F_1 \) must also have full rank. Hence, \( (F_1W_1)^{-1} = W_1^{-1}F_1^{-1} \) and
\[ \|W_1^{-1}\|_2 \leq \|(F_1W_1)^{-1}\|_2\|F_1\|_2 \leq O(1). \]

(6) Bound the sum for a “similar” initial vector:
Note that for \( \tilde{v}_2 := W_2W_1^{-1}\tilde{v}_{0,1} \), we have
\[ WW_1^{-1}\tilde{v}_{0,1} = \begin{pmatrix} I_2 \\ W_2W_1^{-1} \end{pmatrix} \tilde{v}_{0,1} = \begin{pmatrix} \tilde{v}_{0,1} \\ \tilde{w}_2 \end{pmatrix} \]
and \( \tilde{w}_2 \) is “small”:
\[ \|\tilde{w}_2\|_2 \leq \|W_2\|_2\|W_1^{-1}\|_2\|v_{0,1}\|_2 \leq O(m^{-1})O(1)O(m^\varepsilon) = O(m^\varepsilon^{-1}). \]

By Eq. (10), we have \( A^\text{ref}MW = WD_1 \), where \( D_1 \) is the upper left 2 \( \times \) 2 block of \( D \). Therefore,
\[ h\sum_{k=0}^{\infty} \| W(I_2 - hD_1)^k W_1^{-1} \tilde{v}_{0,1}\|_2 = h\sum_{k=0}^{\infty} \| W(I_2 - hD_1)^k W_1^{-1} \tilde{v}_{0,1}\|_2 \leq \|W\|_2\|W_1^{-1}\|_2\|\tilde{v}_{0,1}\|_2 \cdot h\sum_{k=0}^{\infty} \|(I_2 - hD_1)^k\|_2, \]
where
\[ \|W\|_2\|W_1^{-1}\|_2\|\tilde{v}_{0,1}\|_2 \leq O(1)O(1)O(m^\varepsilon) = O(m^\varepsilon) \]
and we can compute the remaining sum similar to step (2):
\[ h\sum_{k=0}^{\infty} \|(I_2 - hD_1)^k\|_2 = h\sum_{k=0}^{\infty} (1 - h\lambda_2(H))^k \leq h \frac{1}{1 - (1 - h\lambda_2(H))} \leq O(m^{-1}). \]
(7) Bound the original sum:

Using \( \bar{v}_0 = WW^{-1}_1 \bar{v}_{0.1} + \left( \begin{array}{c} 0 \\ \bar{v}_{0.2} - \bar{v}_2 \end{array} \right) \), we obtain

\[
\frac{1}{\kappa_{\sigma,k}} \leq h \sum_{k=0}^{\infty} \| (I_4 - hA^{\text{ref}}M)^k \bar{v}_0 \|_2 + h \sum_{k=0}^{\infty} \left\| (I_4 - hA^{\text{ref}}M)^k \left( \begin{array}{c} 0 \\ \bar{v}_{0.2} - \bar{v}_2 \end{array} \right) \right\|_2 
\]

\[
\leq \frac{1}{\kappa_{\sigma,k}} \leq h \sum_{k=0}^{\infty} \| (I_4 - hA^{\text{ref}}M)^k WW_1^{-1} \bar{v}_{0.1} \|_2 + h \sum_{k=0}^{\infty} \| (I_4 - hA^{\text{ref}}M)^k \|_2 \cdot (\| \bar{v}_{0.2} \|_2 + \| \bar{v}_2 \|_2) 
\]

\[\square\]

G Training Dynamics

In this section, we investigate how much the weights \( W_k \) change during training, which allows us to prove Theorem 8 at the end of this section. To this end, we first define important terms.

**Definition G.1.** For any sequence \((z_k)_{k \in \mathbb{N}_0}\), define

\[ \Delta_k z := \max_{0 \leq l \leq k} | z_l - z_0 |, \]

where the supremum should be taken element-wise if \( z \) is a vector or a matrix. Moreover, let

\[ \kappa_{u,k} := h \sum_{l=0}^{k} \| u_l \|_{2,\infty}, \quad \tilde{Q} := \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad 1_3 := \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad 1_{3 \times 3} := \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \]

Now, we can state a general result, which resembles a first-order Taylor approximation.\(^8\)

**Proposition G.2.** Let \( k \in \mathbb{N}_0 \), \( \sigma \in \{ \pm 1 \} \) and \( i \in I_\sigma \). Then, with \( | \cdot | \) and \( \leq \) understood component-wise,

\[ \Delta_k \theta_i \leq \kappa_{u,k} \tilde{Q}_i \theta_{i,0} + 2\kappa_{\sigma}^{2} e^{2\kappa_{\sigma}} \| \theta_{i,0} \|_{2,\infty} 1_3 \]

\[ \Delta_k \Sigma_\sigma \leq \kappa_{u,k} (\tilde{Q}_\sigma \Sigma_{\sigma,0} + | \Sigma_{\sigma,0} (\tilde{Q}) | + 8\kappa_{\sigma}^{2} e^{2\kappa_{\sigma}} \| \Sigma_{\sigma,0} \|_{2,\infty} 1_{3 \times 3} \).

**Proof.** The inequality

\[ \| (A + I)^2 - 2A - I \|_{2,\infty} \leq (\|A\|_{2,\infty} + \|I\|_{2,\infty}^2 - 2\|A\|_{2,\infty} - \|I\|_{2,\infty} ) \]

for arbitrary matrices \( A \) looks like an incorrect application of the triangle inequality due to the minus signs. However, it is correct since the subtracted terms exactly match terms in the expansion of the first term (since \( \|I\|_{2,\infty} = 1 \):

\[
\| (A + I)^2 - 2A - I \|_{\infty} = \|A^2 + 2A + I - 2A - I \|_{\infty} = \|A^2\|_{\infty}
\]

\[
\leq \|A\|_{\infty}^2 = \|A\|_{\infty}^2 + 2\|A\|_{\infty} + \|I\|_{\infty} - 2\|A\|_{\infty} - \|I\|_{\infty}
\]

\[
= (\|A\|_{\infty} + \|I\|_{\infty})^2 - 2\|A\|_{\infty} - \|I\|_{\infty} .
\]

We can apply the same trick to obtain bounds on \( | \theta_{i,k} - \theta_{i,0} | \) and \( | \Sigma_{\sigma,k} - \Sigma_{\sigma,0} | \).\(^9\) Define

\[ \tilde{Q}_k := h \sum_{i=0}^{k} Q_{\sigma,i}, \quad \bar{s}_k := h \sum_{i=0}^{k} \| Q_{\sigma,i} \|_{\infty} . \]

\(^8\)In the “first-order term”, the matrices are still sparse. “Higher-order” approximations are not useful for our purpose.

\(^9\)The bound on \( \Delta_k \theta_i \) and \( \Delta_k \Sigma_\sigma \) then follows since the bound is increasing in \( k \).
Since
\[ \theta_{i,k} = (I_3 + hQ_{\sigma,k-1}) \cdots (I_3 + hQ_{\sigma,0}) \theta_{i,0} \]
\[ \Sigma_{\sigma,k} = (I_3 + hQ_{\sigma,k-1}) \cdots (I_3 + hQ_{\sigma,0}) \Sigma_{\sigma,0} (I_3 + hQ_{\sigma,0}) \cdots (I_3 + hQ_{\sigma,k-1}), \]
we find with $1 + x \leq e^x$:
\[
\| \theta_{i,k} - \tilde{Q}_{k-1} \theta_{i,0} - \theta_{i,0} \|_{\infty} \\
\leq (1 + h\|Q_{\sigma,k-1}\|_{\infty}) \cdots (1 + h\|Q_{\sigma,0}\|_{\infty}) \|\theta_{i,0}\|_{\infty} - \tilde{s}_{k-1} \|\theta_{i,0}\|_{\infty} - \|\theta_{i,0}\|_{\infty} \\
\leq (e^{\delta k} - \tilde{s}_{k-1} - 1)\|\theta_{i,0}\|_{\infty}
\]
and similarly
\[
\| \Sigma_{\sigma,k} - \tilde{Q}_{k-1} \Sigma_{\sigma,0} - \Sigma_{\sigma,0} \tilde{Q}_{k-1} - \Sigma_{\sigma,0} \|_{\infty} \\
\leq (1 + h\|Q_{\sigma,k-1}\|_{\infty}) \cdots (1 + h\|Q_{\sigma,0}\|_{\infty}) \|\Sigma_{\sigma,0}\|_{\infty} (1 + h\|Q_{\sigma,0}\|_{\infty}) \cdots (1 + h\|Q_{\sigma,k-1}\|_{\infty}) \\
- (\tilde{s}_{k-1} \|\Sigma_{\sigma,0}\|_{\infty} + \|\Sigma_{\sigma,0}\|_{\infty}\tilde{s}_{k-1} + 1) \\
\leq (e^{2\delta k} - 2\tilde{s}_{k-1} - 1)\|\Sigma_{\sigma,0}\|_{\infty}.
\]
Observe that
\[
e^x - x - 1 = \sum_{k=2}^{\infty} \frac{x^k}{k!} = x^2 \sum_{k=0}^{\infty} \frac{x^k}{(k+2)!} \leq \frac{1}{2} x^2 \sum_{k=0}^{\infty} \frac{x^k}{k!} = \frac{1}{2} x^2 e^x.
\]
Obviously,
\[
|\tilde{Q}_k| \leq h \sum_{l=0}^{k} |Q_{\sigma,l}| = h \left( \begin{array}{ccc} 0 & 0 & \sum_{l=0}^{k} |r_{\sigma,l}| \\ 0 & 0 & \sum_{l=0}^{k} |s_{\sigma,l}| \\ \sum_{l=0}^{k} |r_{\sigma,l}| & \sum_{l=0}^{k} |s_{\sigma,l}| & 0 \end{array} \right) \leq \kappa_{u,k} \tilde{Q}_k.
\]
We also have $\tilde{s}_k \leq 2\kappa_{u,k}$ since
\[
\|Q_{\sigma,l}\|_{\infty} = \max_{i \in \{1, \ldots, 3\}} \sum_{j=1}^{3} |(Q_{\sigma,l})_{ij}| = |r_{\sigma,l}| + |s_{\sigma,l}| \leq 2\|u_t\|_{\infty}.
\]
Aggregating the previous results and using $\kappa_{u,k-1} \leq \kappa_{u,k}$ yields
\[
|\theta_{i,k} - \theta_{i,0}| \leq |\tilde{Q}_{k-1}||\theta_{i,0}| + |\theta_{i,k} - \tilde{Q}_{k-1} \theta_{i,0} - \theta_{i,0}|_{\infty} \mathbf{1}_3 \\
\leq \kappa_{u,k} \tilde{Q} \|\theta_{i,0}\| + 2\kappa_{u,k}^2 e^{2\kappa_{u,k}} \|\theta_{i,0}\|_{\infty} \mathbf{1}_3.
\]
\[
|\Sigma_{\sigma,k} - \Sigma_{\sigma,0}| \leq |\tilde{Q}_{k-1}||\Sigma_{\sigma,0}| + |\Sigma_{\sigma,0}||\tilde{Q}_{k-1} - \Sigma_{\sigma,0}| \\
+ |\Sigma_{\sigma,0} - \tilde{Q}_{k-1} \Sigma_{\sigma,0} - \Sigma_{\sigma,0} \tilde{Q}_{k-1} - \Sigma_{\sigma,0}|_{\infty} \mathbf{1}_{3 \times 3} \\
\leq \kappa_{u,k} (\tilde{Q} \|\Sigma_{\sigma,0}\| + \|\Sigma_{\sigma,0}\|\tilde{Q} + 8\kappa_{u,k}^2 e^{4\kappa_{u,k}} \|\Sigma_{\sigma,0}\|_{\infty} \mathbf{1}_{3 \times 3}.
\]

**Corollary G.3.** Let Assumption F.2 be satisfied. If $\kappa_{u,k} \leq O(m^{\varepsilon + \gamma_{\psi} - 1})$ for some $k \in \mathbb{N}_0$ with bound independent of $k$, we have
\[
\Delta_k \theta_i \leq O(m^{2\varepsilon + \gamma_{\psi}}) \begin{pmatrix} O(m^{-3/2}) & O(m^{-3/2}) \\ O(m^{-3/2}) & O(m^{-1}) \end{pmatrix},
\]
\[
\Delta_k \Sigma_{\sigma} \leq O(m^{2\varepsilon + \gamma_{\psi}}) \begin{pmatrix} O(m^{-1}) & O(m^{-1}) & O(1) \\ O(m^{-1}) & O(m^{-1}) & O(m^{-1}) \end{pmatrix}
\]
with a bound independent of $k$.

**Proof.** Note that since $\varepsilon + \gamma_{\psi} < 1$, we have $e^{4\kappa_{u,k}} = O(1)$.
(a) By properties (W1), (W2), and (W3) in Proposition E.3 we have
\[ |\theta_{i,0} - \theta_{\ast,0}| = \begin{pmatrix} |a_{i,0}| \\ |b_{i,0}| \\ |w_{i,0}| \end{pmatrix} \leq \begin{pmatrix} m^\varepsilon \\ 0 \\ m^{-1/2} \end{pmatrix}. \]

We can now apply Proposition G.2 to obtain
\[ |\theta_{i,k} - \theta_{\ast,0}| \leq \kappa_{u,k} \|\theta_{i,0}\| + 2\kappa_{u,k}^2 \varepsilon^{2\kappa_{u,k}} \|\theta_{i,0}\| \leq \kappa_{u,k} \left( \frac{m^{\varepsilon-1/2}}{m^\varepsilon} \right) \leq O(m^{2\varepsilon+\gamma_\psi}) \left( \left( O(m^{-3/2}) \atop O(m^{-3/2}) \atop O(m^{-1}) \right) + O(m^{\varepsilon+\gamma_\psi}) \left( O(m^{-2}) \atop O(m^{-2}) \atop O(m^{-1}) \right) \right) \]
\[ \varepsilon + \gamma_\psi \leq 1/2 \]
\[ \leq O(m^{2\varepsilon+\gamma_\psi}) \left( O(m^{-3/2}) \atop O(m^{-3/2}) \atop O(m^{-1}) \right). \]

(b) By properties (W1), (W5), (W6) and (W7) in Proposition E.3 we have
\[ |\Sigma_{\sigma,0}| = \begin{pmatrix} |\Sigma_{\sigma,a^2,0}| & |\Sigma_{\sigma,ab,0}| & |\Sigma_{\sigma,wa,0}| \\ |\Sigma_{\sigma,ab,0}| & |\Sigma_{\sigma,b^2,0}| & |\Sigma_{\sigma,wb,0}| \\ |\Sigma_{\sigma,wa,0}| & |\Sigma_{\sigma,wb,0}| & |\Sigma_{\sigma,w^2,0}| \end{pmatrix} = \begin{pmatrix} O(m) & 0 & O(m^\varepsilon) \\ O(m^\varepsilon) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \]

Since \( \varepsilon, 1 \), we can conclude \( \|\Sigma_{\sigma,0}\|_\infty = O(m) \) and
\[ \tilde{Q}|\Sigma_{\sigma,0}| + |\Sigma_{\sigma,0}||\tilde{Q} = \begin{pmatrix} O(m^\varepsilon) & 0 & O(1) \\ O(m^\varepsilon) & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} O(m^\varepsilon) & O(m^\varepsilon) & O(m) \\ O(m^\varepsilon) & O(m^\varepsilon) & O(m) \\ 0 & 0 & 0 \end{pmatrix} \]
\[ = \begin{pmatrix} O(m^\varepsilon) & O(m^\varepsilon) & O(m) \\ O(m^\varepsilon) & O(m^\varepsilon) & O(m) \\ O(m) & O(1) & O(m^\varepsilon) \end{pmatrix}. \]

We can now apply Proposition G.2 to obtain
\[ |\Sigma_{\sigma,k} - \Sigma_{\sigma,0}| \leq \kappa_{u,k}(\tilde{Q}|\Sigma_{\sigma,0}| + |\Sigma_{\sigma,0}||\tilde{Q}) + 8\kappa_{u,k}^2 \varepsilon^{2\kappa_{u,k}} \|\Sigma_{\sigma,0}\|_\infty \leq O(m^{2\varepsilon+\gamma_\psi}) \left( \begin{pmatrix} 0 & O(m^{-1}) & O(1) \\ O(m^{-1}) & 0 & O(m^{-1}) \\ O(m^{-1}) & O(m^{-1}) & 0 \end{pmatrix} + O(m^{\varepsilon+\gamma_\psi-2}) \right) \]
\[ \varepsilon + \gamma_\psi \leq 1/2 \]
\[ \leq O(m^{2\varepsilon+\gamma_\psi}) \left( \begin{pmatrix} 0 & O(m^{-1}) & O(1) \\ O(m^{-1}) & 0 & O(m^{-1}) \\ O(m^{-1}) & O(m^{-1}) & 0 \end{pmatrix} \right). \]

**Remark G.4.** We will prove in Proposition G.6 that the assumption of Corollary G.3 is satisfied. Although the first inequality of Corollary G.3 already provides bounds on the change of the individual weights, the second inequality is interesting as well because its bounds are stronger than what one would expect only from the individual weight bounds in the first inequality: For the sake of simplicity, pretend that \( \varepsilon = \gamma_\psi = 0 \). Then, for example, one could argue using the first inequality that
\[ \Delta_k \Sigma_{\sigma,0}^2 = \max_{0 \leq l \leq k} \sum_{i \in I_0} (a_{i,l}^2 - a_{i,0}^2) \leq \sum_{i \in I_0} \max_{0 \leq l \leq k} a_{i,l}^2 - a_{i,0}^2 \leq \sum_{i \in I_0} \max_{0 \leq l \leq k} a_{i,l} + a_{i,0} \cdot |a_{i,l} - a_{i,0}| \]
\[ \leq \sum_{i \in I_0} (|a_{i,0}| + \Delta_k a_i) \Delta_k a_i \leq \sum_{i \in I_0} (O(1) + O(m^{-3/2})O(m^{-3/2}) = |I_0|O(m^{-3/2}) \leq O(m^{-1/2}), \]
where $δ$ will be crucial in proving that the assumption $κ_{u,k} ≤ O(m^{ε + γ_φ - 1})$ of Corollary G.3 is satisfied. Also, note that for $ε = γ_φ = 0$, the weakest bound
\[ \Delta_k Σ_{σ,u} = O(1) \]
cannot be improved: $Σ_{σ,u} = p_σ$ is the slope of $f_{w,τ,s}$, which initially satisfies $|Σ_{σ,u,0}| ≤ O(1)$ by (W7) and needs to converge to an $p_σ^{opt}$ that is independent of $Σ_{σ,u,0}$ and also satisfies $|p_σ^{opt}| ≤ ψ_{D,p} ≤ O(1)$. Our proof works since $Σ_{σ,u}$ only occurs in $hG^{Wab}$ with a small factor $h$, but neither in $G^w$ nor $G^{ab}$.

We will soon use Corollary G.3 to prove its own assumption $κ_{u,k} = O(m^{ε + γ_φ - 1})$. To this end, we first need a lemma that connects the reference system $δ\overrightarrow{v} = -hA^{σab}\overrightarrow{w}$ to the actual system $δ\overrightarrow{v} = -hA\overrightarrow{w}$.

**Lemma G.5.** For $m ≥ 1$, let $∥·∥$ denote an arbitrary vector norm on $\mathbb{R}^m$ and its induced matrix norm. Let $k ∈ \mathbb{N}_0$, $K_0, \ldots, K_{k-1} ∈ \mathbb{R}^{m×m}$ and $\hat{K} ∈ \mathbb{R}^{m×m}$. If
\[ δ_{k-1} := \sum_{l=0}^{k-1} ∥\hat{K}^l∥ \cdot \sup_{l ∈ \{0, \ldots, k-1\}} ∥K_l - \hat{K}∥ < 1 \]
then each sequence $v_{l+1} = K_lv_l$ for all $l ∈ \{0, \ldots, k-1\}$ satisfies
\[ ∑_{l=0}^{k} ∥v_l∥ ≤ \frac{1}{1 - δ_{k-1}} ∑_{l=0}^{k} ∥\hat{K}^l v_0∥ \]

**Proof.** Clearly, for $l ∈ \{0, \ldots, k-1\}$,
\[ v_{l+1} = \hat{K}v_l + (K_l - \hat{K})v_l \]
and hence, by induction on $l$,
\[ v_l = \hat{K}v_0 + \sum_{l'=0}^{l-1} \hat{K}^{l-1-l'}(K_{l'} - \hat{K})v_{l'} \]
for all $l ∈ \{0, \ldots, k\}$. Summing norms on both sides yields
\[ ∑_{l=0}^{k} ∥v_l∥ ≤ ∑_{l=0}^{k} ∥\hat{K}^l v_0∥ + ∑_{l=0}^{k} ∑_{l'=0}^{l-1} ∥\hat{K}^{l-1-l'}(K_{l'} - \hat{K})v_{l'}∥ \]
\[ = ∑_{l=0}^{k} ∥\hat{K}^l v_0∥ + ∑_{l=0}^{k} ∑_{l'=0}^{l-1} ∥\hat{K}^{l-1-l'}(K_{l'} - \hat{K})v_{l'}∥ \]
\[ ≤ ∑_{l=0}^{k} ∥\hat{K}^l v_0∥ + ∑_{l=0}^{k} ∑_{l'=0}^{l-1} ∥\hat{K}^{l-1-l'}∥ \cdot \sup_{l ∈ \{0, \ldots, k-1\}} ∥K_l - \hat{K}∥ \cdot ∥v_{l'}∥ \]
\[ ≤ ∑_{l=0}^{k} ∥\hat{K}^l v_0∥ + δ_{k-1} ∑_{l'=0}^{k} ∥v_{l'}∥ \]
Hence $(1 - δ_{k-1}) ∑_{l=0}^{k} ∥v_l∥ ≤ ∑_{l=0}^{k} ∥\hat{K}^l v_0∥$ and since $δ_{k-1} < 1$, the inequality is preserved when dividing by $1 - δ_{k-1}$. □

**Proposition G.6.** Let Assumption F.Z be satisfied. We have
\[ κ_{u,k} ≤ O(m^{ε + γ_φ - 1}) \]
where $κ_{u,k}$ was defined in Definition G.1 and the bound $O(m^{ε + γ_φ - 1})$ is independent of $k ∈ \mathbb{N}_0$. 

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Proof. By Proposition C.5, we know that $\bar{v}_{k+1} = (I_4 - h A_{k} M_D) \bar{v}_{k}$. We want to bound $\kappa_{u,k} = h \sum_{l=0}^{k} \| u_l \|_{\infty} = h \sum_{l=0}^{k} \| B M_D \bar{v}_l \|_{\infty}$ by comparing it to the reference system $\delta \bar{v} = -h A^\text{ref} M_D \bar{v}$ using Lemma G.5. Hence, we define

$$
\delta_k := \sum_{l=0}^{k} \| (I_4 - h A^\text{ref} M_D)^{\lambda} \|_{\infty} \cdot \sup_{0 \leq l \leq k} \| (I_4 - h A^\text{ref} M_D) - (I_4 - h A_{l} M_D) \|_{\infty}
$$

$$
= h \sum_{l=0}^{k} \| (I_4 - h A^\text{ref} M_D)^{\lambda} \|_{\infty} \cdot \sup_{0 \leq l \leq k} \| (A_{l} - A^\text{ref}) M_D \|_{\infty} .
$$

(12)

For $m$ large enough, we want to prove by induction that $\delta_k \leq 1/2$ for all $k \in \mathbb{N}_0$. Trivially, $\delta_{-1} = 0 \leq 1/2$. Now let $k \in \mathbb{N}_0$ with $\delta_{k-1} \leq 1/2$.

(1) By Lemma C.4, we have $\bar{u}_k = -B M_D \bar{v}_k$ and hence $u_k = -B M_D \bar{v}_k$. Thus,

$$
\kappa_{u,k} = h \sum_{l=0}^{k} \| u_l \|_{\infty} \leq \| B \|_{\infty} \| M_D \|_{\infty} \cdot h \sum_{l=0}^{k} \| \bar{v}_l \|_{\infty} .
$$

Because $\delta_{k-1} \leq 1/2$, we can apply Lemma G.5 and obtain

$$
h \sum_{l=0}^{k} \| \bar{v}_l \|_{\infty} \leq \frac{1}{1 - \frac{1}{2}} \cdot \sum_{l=0}^{\infty} \| (I_4 - h A^\text{ref} M_D)^{\lambda} \|_{\infty} \| \bar{v}_0 \|_{\infty}
$$

$$
\leq 2h \sum_{l=0}^{\infty} \| (I_4 - h A^\text{ref} M_D)^{\lambda} \|_{\infty} \| \bar{v}_0 \|_{\infty}
$$

$$
\leq O(m^{\varepsilon + \gamma_\varphi - 1}) .
$$

Norm equivalence (cf. Definition A.3) yields

$$
\| M_D \|_{\infty} \leq O(\| M_D \|_{2}) = O(\lambda_{\max}(M_D)) \leq O(1) .
$$

(13)

Hence, we can write

$$
\kappa_{u,k} = O(m^{\varepsilon + \gamma_\varphi - 1}) ,
$$

(14)

where, in accordance with Definition A.2, the constant in $O(m^{\varepsilon + \gamma_\varphi - 1})$ does not depend on the induction step $k$.

(2) Let us investigate the components of Eq. (12):

$$
h \sum_{l=0}^{k} \| (I_4 - h A^\text{ref} M_D)^{\lambda} \|_{\infty} \leq h \sum_{l=0}^{\infty} \| (I_4 - h A^\text{ref} M_D)^{\lambda} \|_{\infty} = O(1)
$$

$$
(A_{l} - A^\text{ref}) M_D = B \left( (G_{l}^w - G_{0}^w) + (G_{l}^{ab} - G_{0}^{ab}) + h G_{l}^{wab} \right) B M_D
$$

$$
\Rightarrow \| (A_{l} - A^\text{ref}) M_D \|_{\infty} \leq O(1) \cdot (\| G_{l}^w - G_{0}^w \|_{\infty} + \| G_{l}^{ab} - G_{0}^{ab} \|_{\infty} + h \| G_{l}^{wab} \|_{\infty} ) .
$$

First of all, for $0 \leq l \leq k$,

$$
\| G_{l}^w - G_{0}^w \|_{\infty} \leq \max_{\sigma \in \{ \pm \}} \Delta_{k} \Sigma_{\sigma, w^2} \leq O(m^{2\varepsilon + \gamma_\varphi - 1}) .
$$

Similarly, for $0 \leq l \leq k$,

$$
\| G_{l}^{ab} - G_{0}^{ab} \|_{\infty} \leq \max_{\sigma \in \{ \pm \}} (\Delta_{k} \Sigma_{\sigma, a^2} + \Delta_{k} \Sigma_{\sigma, ab} + \Delta_{k} \Sigma_{\sigma, b^2}) \leq O(m^{2\varepsilon + \gamma_\varphi - 1}) .
$$

Observe that

$$
h | r_{\sigma, l} | \leq h \| u_l \|_{\infty} \leq h \sum_{l=0}^{k} \| u_{l}^{\prime} \|_{\infty} = \kappa_{u,k} \leq O(m^{\varepsilon + \gamma_\varphi - 1})
$$

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and similarly $h|s_{\sigma,l}| = O(m^{\varepsilon+\gamma \psi-1})$. Thus, we find

$$h\|G_i^{wab}\|_{\infty} = \max_{\sigma \in \{\pm\}} h|r_{\sigma,i}\Sigma_{\sigma,wa,l} + s_{\sigma,l}\Sigma_{\sigma,wb,l}| = O(m^{\varepsilon+\gamma \psi-1}) \cdot \left(\max_{\sigma \in \{\pm\}} |\Sigma_{\sigma,wa,l}| + |\Sigma_{\sigma,wb,l}|\right).$$

Similar to the other calculations, we can compute for $0 \leq l \leq k$

$$|\Sigma_{\sigma,wa,l}| \leq |\Sigma_{\sigma,wa,0}| + \Delta_k \Sigma_{\sigma,wa} \leq O(m^{\varepsilon}) + O(m^{2\varepsilon+\gamma \psi}) = O(m^{2\varepsilon+2\gamma \psi}),$$

$$|\Sigma_{\sigma,wb,l}| \leq |\Sigma_{\sigma,wb,0}| + \Delta_k \Sigma_{\sigma,wb} \leq 0 + O(m^{2\varepsilon+\gamma \psi-1}) = O(m^{2\varepsilon+\gamma \psi-1}),$$

which yields $h\|G_i^{wab}\|_{\infty} = O(m^{3\varepsilon+2\gamma \psi-1})$.

We can now revisit the beginning of step (2) and obtain $\|(A_l - A^{ref})M_D\|_{\infty} = O(m^{3\varepsilon+2\gamma \psi-1})$ and

$$\delta_k \geq \frac{1}{2} h \sum_{l=0}^{k} \|\left(I_A - hA^{ref}M_D\right)^{l}\|_{\infty} \cdot \sup_{0 \leq l \leq k} \|\left(A_l - A^{ref}\right)M_D\|_{\infty} = O(1) \cdot O(m^{3\varepsilon+2\gamma \psi-1}) = O(m^{3\varepsilon+2\gamma \psi-1}).$$

We have shown that $\delta_{k-1} \leq 1/2$ implies $\delta_k \leq O(m^{3\varepsilon+2\gamma \psi-1})$, where the constant in $O(m^{3\varepsilon+2\gamma \psi-1})$ does not depend on $k$. Since $3\varepsilon + 2\gamma \psi < 1$ by Assumption F.2, we have $\lim_{m \to \infty} m^{3\varepsilon+2\gamma \psi-1} = 0$ and there exists $m_0 \in \mathbb{N}_0$ such that for all $m \geq m_0$ and $k \in \mathbb{N}_0$, $\delta_{k-1} \leq 1/2$ implies $\delta_k \leq 1/2$ and the induction works. Thus, for all $m \geq m_0$ and $k \in \mathbb{N}_0$, we know that $\delta_{k-1} \leq 1/2$ and we can apply step (1) to obtain

$$\kappa_{a,k} = O(m^{\varepsilon+\gamma \psi-1}).$$

We can now prove our main theorem:

**Proof of Theorem 8** Since $\gamma \psi + \gamma_{data} + \gamma P < 1/2$, we can assume without loss of generality that

$$0 < \varepsilon < \frac{1/2 - (\gamma \psi + \gamma_{data} + \gamma P)}{3}.$$

Moreover, if (W1) – (W7) from Proposition E.3 are satisfied, we have (similar to Eq. (7) in the proof of Proposition F.4)

$$\lambda_{\max}(H) = \max\{M_D^{1/2}A^{ref}M_D^{1/2}\} \leq \|M_D^{1/2}\|_2 \lambda_{\max}(A^{ref}) = \lambda_{\max}(M_D)\lambda_{\max}(A^{ref}) \leq K_M\Theta(m).$$

Hence, there exists a constant $C_{U}^{-1} > 0$ with $\lambda_{\max}(H) \leq C_{U}^{-1}m$. For this choice, assumption (e) yields

$$h \leq C_{U}m^{-1} \leq \frac{1}{\lambda_{\max}(H)}.$$ 

Therefore, Assumption F.2 is satisfied whenever the initialization satisfies (W1) – (W7).

By our choice of $\varepsilon$, we have

$$2\varepsilon + \gamma \psi - 3/2 < -1 - \gamma P - \gamma_{data} \leq -1 - \gamma P.$$

For $\varepsilon := K_{data}m^{-\gamma_{data}}$, we then obtain using (W4), Corollary G.3 and Proposition G.6

$$|(a_{i,0} - a_{i,0} - a_{i,k})| \geq \left(\Omega(m^{-1-\gamma P}) - O(m^{2\varepsilon+\gamma \psi-3/2})\right)\Theta(m^{-\gamma_{data}}) \quad \text{and} \quad |b_{i,k}| = |b_{i,k} - b_{i,0}| \leq O(m^{2\varepsilon+\gamma \psi-3/2}).$$

Using (15) again, we find that there exists $m_0$ such that for all $m \geq m_0$ and all $i \in I, k \in \mathbb{N}_0$,

$$|b_{i,k}| < (|a_{i,0} - a_{i,0} - a_{i,k})| \varepsilon,$$
which, in terms of Lemma B.2, means $W_k \in S_{W_0}(x)$. Since $x \leq x_D$ by assumption, we also have $W_k \in S_{W_0}(x_D)$. But then, Lemma B.2 tells us that $\nabla L_{D, \tau}(W_k) = \nabla L_D(W_k)$ and that $f_W|_{|x, \infty|} = f_{W, \tau, 1}|_{|x, \infty|}$ as well as $f_W|_{(-\infty, -2]} = f_{W, \tau, -1}|_{(-\infty, -2]}$ are affine. Hence, $(W_k)_{k \in \mathbb{N}_0}$ satisfies the original gradient descent iteration

$$W_{k+1} = W_k - h \nabla L_D(W_k)$$

and (v) is satisfied. Moreover, by Corollary G.3, we obtain (i), (ii) and (iii) (up to a factor 2 in front of $\varepsilon$, which can be resolved by shrinking $\varepsilon$):

$$|a_{i,k} - a_{i,0}| \leq O(m^{2c+\gamma} - 3/2)$$

$$|b_{i,k} - b_{i,0}| \leq O(m^{2c+\gamma} - 3/2)$$

$$|w_{i,k} - w_{i,0}| \leq O(m^{2c+\gamma} - 1) .$$

In order to find a similar bound for $c$, we recall from Lemma C.4 that $\delta c = h(\hat{s}_1 + \hat{s}_{-1})$, from G.1 that $\kappa_{u,k} = h \sum_{l=0}^{k} \|u_l\|_{\infty}$ and from Definition C.1 that

$$u = B \begin{pmatrix} \hat{r}_1 \\ \hat{f}_{-1} \\ \hat{s}_1 \\ \hat{s}_{-1} \end{pmatrix} \text{ and therefore } \begin{pmatrix} \hat{r}_1 \\ \hat{f}_{-1} \\ \hat{s}_1 \\ \hat{s}_{-1} \end{pmatrix} = B^{-1} u ,$$

since $B$ and invertible due to $|\alpha| \neq 1$. Because $B$ is fixed, we therefore obtain

$$|c_k - c_0| \leq \sum_{l=0}^{k-1} |c_{l+1} - c_l| = \sum_{l=0}^{k-1} |\delta c_l| = h \sum_{l=0}^{k-1} |\hat{s}_{1,l} + \hat{s}_{-1,l}| \leq O(\kappa_{u,k})$$

$$\leq O(m^{2c+\gamma} - 1) ,$$

which shows (iv) after rescaling $\varepsilon$.

All of this holds under the assumption that $m \geq m_0$ and (W1) - (W7), where $m_0$ is independent of $W_0, k, h$. By Proposition E.3, the assumption holds with probability $\geq 1 - O(m^{-\gamma'})$.

## H Multi-Dimensional Inputs

In the following, we investigate the case where

- the one-dimensional $x$ values of $D$ are projected onto a line in a $d$-dimensional input space ($d \in \mathbb{N}$), and
- a two-layer neural network with $d$-dimensional input is trained on this (degenerate) dataset.

In Remark H.1, we show that this $d$-dimensional case can be reduced to the case $d = 1$ and hence, comparable conclusions hold:

**Remark H.1.** Let $d \geq 1$ and let $z \in \mathbb{R}^d$ with $\|z\|_2 = 1$. For a dataset $D \in (\mathbb{R} \times \mathbb{R})^n$, we consider an embedded dataset $\tilde{D} = ((z x_1, y_1), \ldots, (z x_n, y_n)) \in (\mathbb{R}^d \times \mathbb{R})^n$ and a neural network function

$$f_{\tilde{W}}(x) := \tilde{c} + \sum_{i=1}^{m} \tilde{w}_i \varphi(\tilde{a}_i x + \tilde{b}_i) .$$

Then,

$$f_{\tilde{W}}(zx) := \tilde{c} + \sum_{i=1}^{m} \tilde{w}_i \varphi(\tilde{a}_i z x + \tilde{b}_i) = \tilde{c} + \sum_{i=1}^{m} \tilde{w}_i \varphi((z^T \tilde{a}_i) x + \tilde{b}_i) = f_{z \tilde{W}}(x) ,$$

where

$$Z \tilde{W} := \begin{pmatrix} z^T \\ \vdots \\ z^T I_m \end{pmatrix} \begin{pmatrix} \tilde{a}_1 \\ \vdots \\ \tilde{a}_m \\ \tilde{b} \\ \tilde{c} \end{pmatrix} = \begin{pmatrix} z^T \tilde{a}_1 \\ \vdots \\ z^T \tilde{a}_m \\ \tilde{b} \\ \tilde{c} \end{pmatrix} \in \mathbb{R}^{3m+1} .$$
If we naturally extend the definition of $L_D$ in the usual way for $d$-dimensional inputs, Eq. (16) yields $L_D^*(\tilde{W}) = L_D(Z\tilde{W})$. Moreover, since $\|z\|_2 = 1$, we have $ZZ^\top = I_{3m+1}$. Using these two insights, we obtain for $W_k := Z\tilde{W}_k$:

$$W_{k+1} = Z\tilde{W}_{k+1} = Z(\tilde{W}_k - h\nabla_{\tilde{W}_k} L_D(\tilde{W}_k)) = Z\tilde{W}_k - hZZ^\top \nabla L_D(Z\tilde{W}_k) = Z\tilde{W}_k - hZZ^\top \nabla L_D(Z\tilde{W}_k) = W_k - h\nabla L_D(W_k).$$

Hence, $(W_k)_{k \in \mathbb{N}_0}$ satisfy the gradient descent equation for the original dataset $D$. Moreover, if we initialize $\tilde{W}_0$ analogous to Assumption 2, i.e.

$$\tilde{b}_i = 0, \quad \tilde{c} = 0, \quad \tilde{w}_i \sim \frac{1}{\sqrt{m}}Z_w, \quad \tilde{a}_i \sim \tilde{Z}_a$$

(17)

with independent variables, then the initial vector $\tilde{W}_0 = Z\tilde{W}_0$ satisfies

$$b_i = \tilde{b}_i = 0, \quad c = \tilde{c} = 0, \quad w_i = \tilde{w}_i \sim \frac{1}{\sqrt{m}}Z_w, \quad a_i = \sum_{l=1}^{d} z_i \tilde{a}_i \sim Z_a$$

with independent variables and suitable $Z_a$. The random variables $(Z_a, \tilde{Z}_w)$ satisfy (Q1) and (Q2) from Assumption 2 (we only need to verify them for $Z_a$):

(Q1) It is well-known that the sum of independent $\mathbb{R}$-valued random variables $X, Y$ with densities $p_X, p_Y$ has density

$$p_{X+Y}(x) = \int_{\mathbb{R}} p_X(x-y)p_Y(y) \, dy.$$ 

Hence, if we know that there exists a bound $B \in (0, \infty)$ with $p_X(x) \leq B$ for all $x \in \mathbb{R}$, then

$$p_{X+Y}(x) \leq B \int_{-\infty}^{\infty} p_Y(y) \, dy = B.$$ 

Moreover, if $p_X$ and $p_Y$ are symmetric, then $p_{X+Y}$ is also symmetric:

$$p_{X+Y}(y) = \int_{\mathbb{R}} p_X(x-y)p_Y(y) \, dy = \int_{\mathbb{R}} p_X(y-x)p_Y(-y) \, dy = \int_{\mathbb{R}} p_X((-x) - y)p_Y(y) \, dy = p_{X+Y}(-x).$$ 

This directly yields (Q1) for $Z_a$.

(Q2) Since $Z_a$ can be written as a linear combination of random variables that satisfy (Q2), $Z_a$ must also satisfy (Q2) by the Minkowski inequality.

By Eq. (16), we obtain

$$f_{\tilde{W}_k}(zx) = f_{\tilde{W}_k}(x)$$

for all $k \in \mathbb{N}_0$ and $x \in \mathbb{R}$. Especially, we can apply Theorems \[8,10] and \[19] and obtain that under the assumptions of these theorems, the kinks of $x \mapsto f_{\tilde{W}_k}(zx)$ do not cross the data points with high probability.

Since the assumptions of the theorems are (up to modifying constants) invariant under multiplying the $x_j$ by a positive constant, we can also allow $\|z\|_2 \neq 1$ as long as $z \neq 0$. ▶

I Inconsistency Proofs

In this section, we give proofs of several inconsistency results. First, we prove an useful lemma.

**Lemma I.1.** Let $p_{\text{data}}$ be a bounded distribution on $\mathbb{R} \times \mathbb{R}$ satisfying (P1). For $\delta \geq 0$, define

$$\mathcal{F}_\delta := \{ f : \mathbb{R} \to \mathbb{R} \mid f \text{ affine on } (-\infty, -\delta) \text{ and } (\delta, \infty) \}, \quad R_{p_{\text{data}}, \delta}^* := \inf_{f \in \mathcal{F}_\delta} R_{p_{\text{data}}}(f).$$

Then, $\lim_{\delta \searrow 0} R_{p_{\text{data}}, \delta}^* = R_{p_{\text{data}}, 0}^*$. 

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Proof. In the case $\eta = \infty$, we obviously have $R_{p_{\text{data}}, \delta}^* = R_{p_{\text{data}}, 0}^*$ for all $\delta \geq 0$ with $P_{\text{data}}^X((-\delta, \delta)) = 0$ and we are done.

Obviously, $R_{p_{\text{data}}, \delta}^*$ is non-increasing in $\delta$. To derive a contradiction, assume that $\lim_{\delta \rightarrow 0} R_{p_{\text{data}}, \delta}^* < R_{p_{\text{data}}, 0}^*$.

For $\delta' > 0, \sigma \in \{-1, 1\}$, consider $P_{\sigma} := P_{\text{data}}(\cdot \mid \sigma X \geq \delta')$. For sufficiently small $\delta'$, $P$ is well-defined and $P_X$ is not only concentrated on a single $x$ value due to (P1). Now, fix such a $\delta' > 0$.

For $f \in F_{\delta}$, define $v_f(\delta) \in \mathbb{R}^{2 \times 2}$ as the slope and intercept of $f$ on $\sigma(\delta, \infty)$. As in Definition 7 we can construct an invertible matrix $M_{p_{\sigma}} = M_{p_{\sigma}, \sigma}$ and a vector $v_{p_{\sigma}} = v_{p_{\sigma}, \sigma}$. Analogously to Remark D.5 we obtain for $\delta \leq \delta'$:

$$R_{p_{\sigma}}(f) \geq (v_f(\delta) - v_{p_{\sigma}}) \top M_{p_{\sigma}}(v_f(\delta) - v_{p_{\sigma}}) .$$

Hence, for $f \in F_{\delta}$ with $\delta \leq \delta'$ and $R_{p_{\text{data}}}(f) \leq R_{p_{\text{data}}, 0}^*$, we obtain

$$R_{p_{\text{data}}, 0}^* \geq R_{p_{\text{data}}}(f) \geq \frac{1}{2} E_{(x,y) \sim P_{\text{data}}} I_{[-\delta, \delta]}(x)(y - f(x))^2$$

$$= \frac{1}{2} P_{\text{data}}^X(\sigma(\delta', \infty)) \cdot E_{(x,y) \sim P_{\sigma}}(y - f(x))^2$$

$$\geq \frac{1}{2} P_{\text{data}}^X(\sigma(\delta', \infty)) \cdot (v_f(\delta) - v_{p_{\sigma}}) \top M_{p_{\sigma}}(v_f(\delta) - v_{p_{\sigma}}) .$$

Since $M_{p_{\sigma}} > 0$ and $P_{\text{data}}^X(\sigma(\delta', \infty)) > 0$, there must exist a constant $C$ such that $\|v_f(\delta)\|_{\infty} \geq C$ for all such $f$ and $\sigma \in \{-1, 1\}$.

Now, pick $f \in F_{\delta}$, $0 < \delta \leq \delta'$, with $R_{p_{\text{data}}}(f) \leq R_{p_{\text{data}}, 0}^*$ and let $f_0 \in F_0$ be its affine continuation (i.e. $f_0(x) = f(x)$ for $|x| > \delta$). Then, $|f_0(x)| \leq C(1 + |x|)$ for $x > 0$ and therefore

$$R_{p_{\text{data}}, 0}^* \leq R_{p_{\text{data}}}(f_0) \geq \frac{1}{2} E_{(x,y) \sim P_{\text{data}}} I_{[-\delta, \delta]}(x)(y - f_0(x))^2$$

$$\geq \frac{1}{2} E_{(x,y) \sim P_{\text{data}}} I_{[-\delta, \delta]}(x)(y - f_0(x))^2 + \frac{1}{2} E_{(x,y) \sim P_{\text{data}}} I_{[-\delta, \delta]}(x)^2$$

$$\rightarrow 0 \quad (\delta \rightarrow 0)$$

Since we can choose $R_{p_{\text{data}}}(f)$ arbitrarily close to $R_{p_{\text{data}}, \delta}^*$, it follows that $R_{p_{\text{data}}, 0}^* \leq \lim_{\delta \rightarrow 0} R_{p_{\text{data}}, \delta}^*$, which contradicts our initial assumption. 

We can now prove various inconsistency results:

Proof of Corollary 21. Let $\gamma_\psi \in (0, 1/2)$ be sufficiently large such that $\frac{1}{\gamma_\psi - 2r_{\text{opt}}} \geq 1 - \varepsilon$. We can then choose $K_{\text{param}} > 0$ sufficiently large such that

$$m_n \leq K_{\text{param}} n^{\frac{3 - \gamma_\psi}{2 - 2r_{\text{opt}}}}$$

for all $n \geq 1$. Choose $K_{\text{data}} > 0$ such that $P_{\text{data}}^X([-K_{\text{data}}, K_{\text{data}}]) = 0$. Moreover, let $\gamma_{\text{data}} = 0$ and $\gamma_P > 0$ such that $\gamma_P + \gamma_{\text{data}} + \gamma_\psi < 1/2$.

Let $C_\psi$ be the corresponding constant from Theorem 19. Since $m_n \rightarrow \infty$ and $h_n < o(m_n^{-1})$, there exists an $n_0$ such that for all $n \geq n_0$, we have

$$h_n \leq C_\psi m_n^{-1} .$$

By Theorem 19 we hence obtain for all $n \geq n_0$ that $f_{W_k}$ is affine on $(-\infty, -K_{\text{data}})$ and $[K_{\text{data}}, \infty)$ with probability $\geq 1 - C_P n^{-\gamma_P} \rightarrow 1$ ($n \rightarrow \infty$). But such a function satisfies $f_{W_k} \in F_{K_{\text{data}}}$ and, because $P_{\text{data}}^X([-K_{\text{data}}, K_{\text{data}}]) = 0$, we obtain

$$R_{p_{\text{data}}}(f_{W_k}) \geq R_{p_{\text{data}}, K_{\text{data}}}^* = R_{p_{\text{data}}, 0}^* \geq R_{p_{\text{data}}, 0}^* ,$$

which yields inconsistency. 

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Proof of Corollary 22. Consider an NN as in Corollary 21 that is inconsistent on a distribution \(P_{\text{data}}\) on \(\mathbb{R} \times \mathbb{R}\). Furthermore, fix an arbitrary vector \(z \in \mathbb{R}^d\) with \(\|z\|_2 = 1\).

For \((x, y) \sim P_{\text{data}}\), let \(\tilde{P}_{\text{data}}\) denote the distribution of \((xz, y)\). It is easy to show that the optimal population risks satisfy

\[
R_{\tilde{P}_{\text{data}}}^* = R_{P_{\text{data}}}^*. \tag{18}
\]

Let \(D \sim (P_{\text{data}})^n\), i.e. \(D\) consists of \(n\) i.i.d. data points \((x_j, y_j) \sim P_{\text{data}}\), then \(\tilde{D} \sim (\tilde{P}_{\text{data}})^n\) with \(\tilde{D}\) defined in Remark H.1. Let \(W_0\) be independent from \(\tilde{D}\) and initialized analogous to Assumption 2 as discussed in Remark H.1. Let

\[
\tilde{W}_{k+1} = \tilde{W}_k - h_n \nabla L_{\tilde{D}}(\tilde{W}_k).
\]

Let \(W_k := Z\tilde{W}_k\). As shown in Remark H.1 \(W_0\) satisfies Assumption 2 and \((W_k)_{k \in \mathbb{N}_0}\) arises from gradient descent on \(D\):

\[
W_{k+1} = W_k - h_n \nabla L_D(W_k).
\]

Moreover, \(f_{\tilde{W}_k}(xz) = f_{W_k}(x)\) for all \(x \in \mathbb{R}, k \in \mathbb{N}_0\) and therefore

\[
R_{\tilde{P}_{\text{data}}}(f_{\tilde{W}_k}) = R_{P_{\text{data}}}(f_{W_k}) \tag{19}
\]

for all \(k \in \mathbb{N}_0\). Since the NN with one-dimensional input is inconsistent on \(P_{\text{data}}\), the NN with \(d\)-dimensional input must be inconsistent on \(\tilde{P}_{\text{data}}\) by (18) and (19).

\[\square\]

Theorem I.2 (Inconsistency for \(\eta < \infty\)). Let \(P_{\text{data}}\) satisfy Assumption 13 for some \(\eta \in (4, \infty)\). Consider an NN estimator as in Corollary 21, but with \(m_n = \Theta(n^{\gamma})\) for \(\frac{2}{\eta} < \gamma < 1 - \frac{2}{\eta}\). Then, this NN estimator is inconsistent for \(P_{\text{data}}\).

Proof. Since

\[
\frac{1}{\gamma \eta} < \frac{1}{2}, \quad 1 - \frac{1}{2\gamma} + \frac{1}{\eta \gamma} = 1 - \frac{1 - \frac{2}{\eta}}{2\gamma} = \frac{2\gamma - \left(1 - \frac{2}{\eta}\right)}{2\gamma} < \frac{1}{2},
\]

there exist some

\[
\gamma_{\psi} \geq \max \left\{ 0, 1 - \frac{1}{2\gamma} \right\}, \quad \gamma_{\text{data}} > \frac{1}{\gamma \eta}, \quad \gamma_P > 0
\]

such that \(\gamma_{\psi} + \gamma_{\text{data}} + \gamma_P < 1/2\). We then have

\[
\gamma \leq \frac{1}{2 - 2\gamma_{\psi}}, \quad 1 - \gamma \eta \gamma_{\text{data}} < 0
\]

and therefore

\[
m_n \leq O \left( n^{\frac{1}{2 - 2\gamma_{\psi}}} \right), \quad O(n^{1 - \gamma_{\text{data}}}) = o(1), \quad O(m_n^{-\gamma_P}) = o(1). \]

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Let $C_h$ be the corresponding constant from Theorem 19. Since $m_n \to \infty$ and $h_n < o(m_n^{-1})$, there exists an $n_0$ such that for all $n \geq n_0$, we have

$$h_n \leq C_h m_n^{-1}.$$ 

Hence, by Theorem 19, we obtain for all $n \geq n_0$ that $f_{W_k} \in F_{K_{\text{data}} m_n^{-\gamma_{\text{data}}}}$ with probability $\geq 1 - C_P (m_n^{-\gamma_P} + nm_n^{-\gamma_{\text{data}}}) \to 1$ for $n \to \infty$. By assumption (P4), we have $R_{p_{\text{data}}, \beta}^* > R_{p_{\text{data}}}^*$ and by Lemma I.1 there exists $\delta > 0$ such that $R_{p_{\text{data}}, \beta}^* > R_{p_{\text{data}}}^*$. For $n$ sufficiently large, we have $K_{\text{data}} m_n^{-\gamma_{\text{data}}} \leq \delta$ and therefore

$$R_{p_{\text{data}}} (f_{W_k}) \geq R_{p_{\text{data}}, \beta}^* > R_{p_{\text{data}}}^*$$

with probability $\geq 1 - C_P (m_n^{-\gamma_P} + nm_n^{-\gamma_{\text{data}}}) \to 1$ for $n \to \infty$. This shows inconsistency. 

\section*{J Miscellaneous}

In this section, we prove a fact that has been mentioned in the main paper.

\textbf{Lemma J.1.} Let $D = ((x_1, y_1), \ldots, (x_n, y_n)) \in (\mathbb{R} \times \mathbb{R})^n$ with $n \geq 1$ and $x_j \neq 0$ for all $j$. Then, by adding three points to $D$, we can achieve that $M_{D, \sigma}$ is invertible for both $\sigma \in \{\pm 1\}$ and that $\psi_{D, q} = 0$.

\textbf{Proof.} By adding at most one point to $D$, we can ensure that both $D_1$ and $D_{-1}$ are nonempty. Now consider the case of $D_1$ ($D_{-1}$ can be handled analogously). For $x' := 1 + \max_{(x, y) \in D_1} x$ and $y' \in \mathbb{R}$ yet to be specified, consider the dataset $\tilde{D} := D \cup \{(x', y')\}$. Since the kernels of two different matrices $M_{x_j} \succeq 0$ and $M_{x'} \succeq 0$ only intersect in zero, we have

$$M_{D_1} = \frac{1}{n+1} \left( M_{x'} + \sum_{(x, y) \in D_1} M_x \right) \succ 0,$$

i.e. $M_{D_1}$ is invertible. Moreover, we have

$$\begin{pmatrix} p_{D_1}^{\text{opt}} \\ q_{D_1}^{\text{opt}} \end{pmatrix} = \begin{pmatrix} v_{D_1}^{\text{opt}} \\ u_{D_1}^{\text{opt}} \end{pmatrix} = M_{D_1}^{-1} \begin{pmatrix} u_{(x', y')} \\ \sum_{(x, y) \in D_1} u_{(x, y)} \end{pmatrix} = \frac{y'}{n+1} M_{D_1}^{-1} \begin{pmatrix} x' \\ 1 \end{pmatrix} + \frac{n}{n+1} M_{D_1}^{-1} u_{D_1}^{\text{opt}}.$$

We need to show that we can choose $y'$ such that $q_{D_1}^{\text{opt}} = 0$. Assume the contrary, which means that there exists $z \in \mathbb{R}$ with

$$M_{D_1}^{-1} \begin{pmatrix} x' \\ 1 \end{pmatrix} = \begin{pmatrix} z' \\ 0 \end{pmatrix} \quad \text{or, equivalently,} \quad \begin{pmatrix} x' \\ 1 \end{pmatrix} = M_{D_1} \begin{pmatrix} z' \\ 0 \end{pmatrix} = \frac{z'}{n+1} \begin{pmatrix} x' \\ 1 \end{pmatrix} + \sum_{(x, y) \in D_1} \begin{pmatrix} x \\ 1 \end{pmatrix}.$$

Since $D_1$ is nonempty by assumption and all $(x, y) \in D_1$ satisfy $x < x'$, we obtain the desired contradiction. Overall, we can therefore satisfy $M_{D, \sigma} \succ 0$ for both $\sigma \in \{\pm 1\}$ by adding at most point to $D$ and we can then satisfy $\psi_{D, q} = 0$ by adding at most two more points to $D$. \qed