LEARNING DEEP LINEAR NEURAL NETWORKS: RIEMANNIAN GRADIENT FLOWS AND CONVERGENCE TO GLOBAL MINIMIZERS

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Abstract. We study the convergence of gradient flows related to learning deep linear neural networks from data (i.e., the activation function is the identity map). In this case, the composition of the network layers amounts to simply multiplying the weight matrices of all layers together, resulting in an overparameterized problem. We show that the gradient flow with respect to these factors can be re-interpreted as a Riemannian gradient flow on the manifold of rank-$r$ matrices endowed with a suitable Riemannian metric. We show that the flow always converges to a critical point of the underlying functional. Moreover, in the special case of an autoencoder, we show that the flow converges to a global minimum for almost all initializations.

1. Introduction

Deep learning [8] forms the basis of remarkable breakthroughs in many areas of machine learning. Nevertheless, its inner workings are not yet well-understood and mathematical theory of deep learning is still in its infancy. Training a neural network amounts to solving a suitable optimization problem, where one tries to minimize the discrepancy between the predictions of the model and the data. One important open question concerns the convergence of commonly used gradient descent and stochastic gradient descent algorithms to the (global) minimizers of the corresponding objective functionals. Understanding this problem for general nonlinear deep neural networks seems to be very involved. In this paper, we study the convergence properties of gradient flows for learning deep linear neural networks from data. While the class of linear neural networks may be not be rich enough for many machine learning tasks, it is nevertheless instructive and still a non-trivial task to understand the convergence properties of gradient descent algorithms. Linearity here means that the activation functions in each layer are just the identity map, so that the weight matrices of all layers are multiplied together. This results in an overparameterized problem.

Our analysis builds on previous works on gradient descent and gradient flows for linear neural networks [15, 10, 9, 3, 7]. In [3] the gradient flow for weight matrices of all network layers is analyzed and an equation for the flow of their product is derived. The article [3] then establishes local convergence for initial points close enough to the (global) minimum. In [7] it is shown that under suitable conditions the flow converges to a critical point for any initial point. We contribute to this line of work in the following ways:

- We show (see Corollary 8) that the evolution of the product of all network layer matrices can be re-interpreted as a Riemannian gradient flow on the manifold of matrices of rank $r$, where $r$ corresponds to the smallest of the involved matrix dimensions. This is remarkable because it is shown in [3] that the flow of this product cannot be interpreted as a standard gradient flow with respect to some functional. Our result is possible because we use a non-trivial Riemannian metric.
- We show that the flow always converges to a critical point of the functional (Theorem 12).
- In the special case of an autoencoder [8, Chapter 14] (which in the linear case is closely related to principal component analysis) and so-called balanced initialization, we show that the flow converges to the global optimum for almost all initializations (Theorem 31). Here, we build on an abstract result in [12] that shows that strict saddle points of the functional are avoided almost surely.

We believe that our results shed new light on global convergence of gradient flows (and thereby on gradient descent algorithms) for learning neural network. We expect that the insights will be useful for extending them to learning nonlinear neural networks.

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Structure. This article is structured as follows. Section 2 describes the setup of gradient flows for learning linear neural networks and collects some basic results. Section 3 provides the interpretation as Riemannian gradient flow on the manifold of rank-\(r\) matrices. Section 4 shows convergence of the flow to a critical point of the functional. For the special case of a linear autoencoder with two coupled layers and balanced initial points, Section 5 shows convergence of the flow to a global optimum for almost all starting points by building on [18]. Section 6 extends this result to autoencoders with an arbitrary number of (non-coupled) layers by first extending an abstract result in [14] that first order methods avoid strict saddle points almost surely to gradient flows and then showing that the strict saddle point property holds for the functional under consideration. Section 7 illustrates our findings with numerical experiments.

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2. Gradient flows for learning linear networks

Suppose we are given data points \(x_1, \ldots, x_m \in \mathbb{R}^{d_x}\) and label points \(y_1, \ldots, y_m \in \mathbb{R}^{d_y}\). Let \(X \in \mathbb{R}^{d_x \times m}\) be the matrix with columns \(x_1, \ldots, x_m\) and let \(Y \in \mathbb{R}^{d_y \times m}\) be the matrix with columns \(y_1, \ldots, y_m\). Let \(N \in \mathbb{N}\) be at least 2, let \(d_1, \ldots, d_{N-1} \in \mathbb{N}\), and let \(d_0 = d_x\) and \(d_N = d_y\). We consider the optimization problem

\[
\min_{W_1, \ldots, W_N} \| Y - W_N \cdots W_1 X \|_F, \quad \text{where } W_j \in \mathbb{R}^{d_j \times d_{j-1}}, \ j = 1, \ldots, N, \tag{1}
\]

Borrowing notation from [3], for \(W_1, \ldots, W_N\) as above, let

\[
L^N(W_1, \ldots, W_N) := \frac{1}{2} \| Y - W_N \cdots W_1 X \|_F^2, \tag{2}
\]

and for \(W \in \mathbb{R}^{d_x \times d_y}\), let

\[
L^1(W) := \frac{1}{2} \| Y - WX \|_F^2. \tag{3}
\]

The mapping \(x \mapsto W_N \cdots W_1 x\) can be referred to as a deep linear network and the factorization

\[
W = W_N \cdots W_1 \tag{4}
\]

as an overparametrization of the matrix \(W\). The optimization problem (1) arises naturally when trying to fit the deep linear network, i.e., the linear map \(W\), to the data so that \(y_\ell \approx W x_\ell, \ \ell = 1, \ldots, m\)

The case of an autoencoder [8, Chapter 14], studied in detail below, refers to the situation where \(r := \min_{i=0, \ldots, N} d_i < m\) is of interest then, as otherwise one could simply set \(W = I_{d_x}\) and there would be nothing to learn.

Note that

\[
\nabla_W L^1(W) = WX^T - YY^T.
\]

For given initial values \(W_j(0), \ j \in \{1, \ldots, N\}\), we consider the system of gradient flows

\[
\dot{W}_j = -\nabla_{W_j} L^N(W_1, \ldots, W_N). \tag{5}
\]

Our aim is to investigate when this system converges to an optimal solution, i.e., one that is minimizing our optimization problem (1). For \(W = W_N \cdots W_1\) we also want to understand the behavior of \(W(t)\) as \(t\) tends to infinity. Clearly, the gradient flow is a continuous version of gradient descent algorithms used in practice and has the advantage that its analysis does not require discussing step sizes etc. We postpone the extension of our results to gradient descent algorithms to later contributions.

Definition 1. Again borrowing notation from [3], for \(W_j \in \mathbb{R}^{d_j \times d_{j-1}}, \ j = 1, \ldots, N\), we say that \(W_1, \ldots, W_N\) are \(0\)-balanced or simply balanced if

\[
W^T_{j+1} W_{j+1} = W_j W_j^T \quad \text{for } j = 1, \ldots, N-1.
\]

We say that the flow (5) has balanced initial conditions if \(W_1(0), \ldots, W_N(0)\) are balanced.

The following lemma summarizes basic properties of the flow. Points (1)-(4) are known; see [4, 8, 11].
Lemma 2. With the notation above, the following holds:

1. For \( j \in \{1, \ldots, N\} \),
   \[
   \nabla_{W_j} L^N(W_1, \ldots, W_N) = W_{j+1}^T \cdots W_N^T \nabla W L^1(W_N \cdots W_1) W_1^T \cdots W_{j-1}^T.
   \]

2. Assume the \( W_j(t) \) satisfy (2). Then \( W = W_N \cdots W_1 \) satisfies
   \[
   \frac{dW(t)}{dt} = - \sum_{j=1}^{N} W_N \cdots W_{j+1} W_{j+1}^T \cdots W_N^T \nabla W L^1(W) W_1^T \cdots W_{j+1}^T W_{j+1} \cdots W_1.
   \]

3. For all \( j = 1, \ldots, N - 1 \) and all \( t \geq 0 \) we have that
   \[
   \frac{d}{dt} \left( W_{j+1}(t) W_{j+1}(t) \right) = \frac{d}{dt} \left( W_j(t) W_j^T(t) \right).
   \]
   In particular, the differences
   \[
   W_{j+1}(t) W_{j+1}(t) - W_j(t) W_j^T(t), \quad j = 1, \ldots, N - 1,
   \]
   are all constant in time.

4. If \( W_1(0), \ldots, W_N(0) \) are balanced, then
   \[
   W_{j+1}(t) W_{j+1}(t) = W_j(t) W_j^T(t)
   \]
   for all \( j \in \{1, \ldots, N - 1\} \) and \( t \geq 0 \), and
   \[
   R(t) := \frac{dW(t)}{dt} + \sum_{j=1}^{N} (W(t) W(t)^T)^{\frac{3}{2}} \nabla W L^1(W(t)) W(t) W(t)^T \frac{dt}{W(t)} = 0.
   \]

5. In the non-balanced case, the term \( R \) defined in (7) satisfies
   \[
   \|R(t)\|_F \leq C \|W(t)\|_{\frac{3}{2}} + \tilde{C},
   \]
   where \( C \) and \( \tilde{C} \) are suitable positive constants depending only on the initial conditions.

6. For any \( i \),
   \[
   \|W_i(t)\|_F \leq C_i \|W(t)\|_F^{\frac{1}{N}} + \tilde{C}_i,
   \]
   where again \( C_i \) and \( \tilde{C}_i \) are suitable positive constants depending only on the initial conditions.

Before we prove the lemma, we introduce the following notation.

Definition 3. Suppose we are given a set of (real valued) matrices \( \{X_i, i \in I\} \), where \( I \) is a finite set. A polynomial \( P \) in the matrices \( X_i, i \in I \) with matrix coefficients is a (finite) sum of terms of the form
\[
A_1 X_{i_1} A_2 X_{i_2} \cdots A_n X_{i_n} A_{n+1}.
\]
The \( A_j \) are the matrix coefficients of the monomial (10) (where the dimensions of the \( A_j \) have to be such that the product (10) as well as the sum of all the terms of the form (10) in the polynomial \( P \) are well defined). The degree of the polynomial \( P \) is the maximal value of \( n \) in the summands of the above form (10) defining \( P \) (where \( n = 0 \) is also allowed).

Proof of Lemma 2. The first four points can be shown by a straightforward calculation and can be found in (4) (5) (7). In the following, the constants are allowed to depend on the dimensions \( d_i \) and the initial matrices \( W_i(0) \). We will suppress the argument \( t \) and split the proof into two steps.

Step 1. For the proof of the statement (6) we observe that
\[
WW^T = W_N \cdots W_1 W_1^T \cdots W_N^T.
\]
Replacing \( W_1 W_1^T \) by \( W_2^T W_2 + A_{12} \), where \( A_{12} \) is a constant matrix (see point (3)), we obtain
\[
WW^T = W_N \cdots W_3 W_2^T W_2 W_2 W_2^T W_3^T \cdots W_N^T + W_N \cdots W_2 A_{12} W_2^T \cdots W_N^T.
\]
Replacing \( W_2W_1^T \) by \( W_3^T W_3 + A_{23} \) and proceeding in this manner, we finally obtain
\[
WW^T = (W_NW_N^T)^N + P(W_2, \ldots, W_N, W_2^T \ldots W_N^T),
\]
where \( P(W_2, \ldots, W_N, W_2^T \ldots W_N^T) \) is a polynomial in \( W_2, \ldots, W_N, W_2^T \ldots W_N^T \) (with matrix coefficients) whose degree is at most \( 2N - 2 \).

In the following, we denote by \( \sigma_N \) the maximal singular value of \( W_N \). Thus
\[
\sigma_N^2 \leq \| (W_NW_N^T)^N \|_F \leq \| WW^T \|_F + \| P(W_2, \ldots, W_N, W_2^T \ldots W_N^T) \|_F.
\]

Since \( \| W_NW_N^T \|_F^2 \) and \( \| W_iW_i^T \|_F^2 \) differ only by a constant (depending on \( i \)), there are suitable constants \( a_i \) and \( b_i \) such that \( \| W_i \|_F \leq a_i\sigma_N + b_i \) for all \( i \in \{1, \ldots, N\} \). It follows that
\[
\| P(W_2, \ldots, W_N, W_2^T \ldots W_N^T) \|_F \leq P_N(\sigma_N),
\]
where \( P_N \) is a polynomial in one variable of degree at most \( 2N - 2 \). Hence we obtain from (12)
\[
\sigma_N^2 \leq B_N \| WW^T \|_F + \tilde{B}_N,
\]
and therefore also
\[
\sigma_N \leq B'_N \| W \|_F^{1/N} + \tilde{B}'_N,
\]
for suitable positive constants \( B_N, \tilde{B}_N, B'_N, \tilde{B}'_N \). Since \( \| W_i \|_F \leq a_i\sigma_N + b_i \), estimate (9) for \( \| W_i \|_F \) follows.

**Step 2.** Now we turn to point (5), i.e., the estimate for \( R \). In the equation
\[
\frac{dW(t)}{dt} = -\sum_{j=1}^N W_N \cdots W_{j+1} W_j^T \cdots W_{N-1} W_{N-1} \cdots W_1,
\]
we replace again recursively the terms \( W_iW_i^T \) on the left of \( \nabla_W L^1(W) \) by \( W_{i+1} W_i + A_{i+1} \), where \( A_{i+1} \) is a constant matrix. Similarly, we replace recursively the terms \( W_i^T W_i \) on the right hand side of \( \nabla_W L^1(W) \) by \( W_{i+1} W_i^T - A_{i+1} \). We finally obtain
\[
\frac{dW(t)}{dt} = -\sum_{j=1}^N (W_NW_N^T)^{N-j} \nabla_W L^1(W)(W_1^T W_1)^{j-1} + F(W_1, \ldots, W_N, W_2^T \ldots W_N^T, \nabla_W L^1(W)), \tag{15}
\]
where \( F(W_1, \ldots, W_N, W_1^T \ldots W_N^T, \nabla_W L^1(W)) \) is a polynomial (with matrix coefficients) in the \( W_i \) and \( W_i^T \) (where \( i = 1, \ldots, N \)) and \( \nabla_W L^1(W) \). Its degree in \( W_1, \ldots, W_N, W_1^T \ldots W_N^T \) (i.e., regarding \( \nabla_W L^1(W) \) as a constant matrix) is at most \( 2N - 4 \). Its degree in \( \nabla_W L^1(W) \) is 1 (each summand of the polynomial contains the factor \( \nabla_W L^1(W) \)). In order to compare the r.h.s. of (15) with the sum in (7), we estimate\(^1\)
\[
\| (W_NW_N^T)^{N-j} \|_{\infty} \leq K_1 \| (W_NW_N^T)^{N-j} \|_F \| WW^T \|_F \| A_{j+1} \|_2 \tag{16}
\]
and
\[
\| (W_1^T W_1)^{j-1} \|_{\infty} \leq K_2 \| (W_1^T W_1)^{j-1} \|_F \| W_1 \|_F \| A_{i+1} \|_2 \tag{17}
\]
for suitable positive constants \( K_1, K_2 \), as follows from (5) Theorem X.1.1. By the proof of point (6) (i.e., equation (11)), for \( j < N \), the norm \( \| (W_NW_N^T)^{N(j-1)} - (WW^T)^{N-j} \|_F \) can be estimated by a polynomial in the \( \| W_i \|_F \) of degree at most \( 2N(N-j) - 2 \). Analogously, for \( j > 1 \), the norm
\[
\| (W_1^T W_1)^{N(j-1)} - (W_1^T W_1)^{j-1} \|_F
\]
can be estimated by a polynomial in the norms \( \| W_i \|_F \) of degree at most \( 2N(j-1) - 2 \). (To see this, write \( W_1^T W_1 = W_1 \cdots W_1^T W_1 \cdots W_1 \), replace recursively the \( W_1^T W_1 \) by \( W_{i+1} W_i^T - A_{i+1} \), and argue analogously to the proof of equation (11).) Using estimate (8), it follows that for \( j < N \)
\[
\| (W_NW_N^T)^{N(N-j)} - (WW^T)^{N-j} \|_F \leq D_1 \| W \|_F^{2(N-j)} + D_2 \tag{18}
\]
and for \( j > 1 \)
\[
\| (W_1^T W_1)^{N(j-1)} - (W_1^T W_1)^{j-1} \|_F \leq D_3 \| W \|_F^{2(j-1)} + D_4 \tag{19}
\]
\(^1\)This theorem states that for any operator monotone function \( f \) on \( (0, \infty) \) with \( f(0) = 0 \) and positive semidefinite matrices \( A, B \) of the same size, we have \( \| f(A) - f(B) \| \leq f(\| A - B \|) \), where \( \| \cdot \| \) denotes the spectral norm. We apply this theorem with \( f(t) = t^{1/N} \) and use the equivalence of the Frobenius norm and the spectral norm given the size of the matrices \( A, B \).
for suitable positive constants $D_i$. Again using \((\ref{eq:grad_est})\) and the fact that $F$ has degree at most $2N - 4$ as a polynomial in the $W_i$ and $W^T_i$ and degree 1 as a polynomial in $\nabla_W L^1(W)$, it follows that
\[
\|F(W_1, \ldots W_N, W^T_1, \ldots W^T_N, \nabla_W L^1(W))\|_F \leq D_5\|W\|_F^{3-\frac{1}{2}} + D_6,
\]
where we have used that
\[
\|\nabla_W L^1(W)\|_F \leq D_7\|W\|_F + D_8.
\]
Again the $D_i$ are suitable positive constants. Writing now
\[
\frac{dW(t)}{dt} = -\sum_{j=1}^N \left( (WW^T)_{i,i} + \left( (W_NW^T_i)^{N-j} - (WW^T)^{i,i} \right) \right) \nabla_W L^1(W)
\]
\[
\times \left( (W^TW)_{j,j} + \left( (W^TW)^{j,j} \right) \right)
\]
\[
+ F(W_1, \ldots W_N, W^T_1, \ldots W^T_N, \nabla_W L^1(W)),
\]
and combining estimates \((\ref{eq:grad_est}), \,(\ref{eq:grad_est2}), \,(\ref{eq:grad_est3}), \,(\ref{eq:grad_est4}), \,(\ref{eq:grad_est5}), \text{ and } \,(\ref{eq:grad_est6}),\) it follows that
\[
\|R\|_F \leq C\|W\|_F^{3-\frac{1}{2}} + \tilde{C}
\]
for suitable positive constants $C, \tilde{C}$.

\begin{definition}
\end{definition}

Definition 4. For $W, Z \in \mathbb{R}^{d_x \times d_z}$ und $N \geq 2$ let
\[
A_W(Z) = \sum_{j=1}^N (WW^T)^{i,i} \cdot Z \cdot (W^TW)^{i,i}.
\]
Thus, if the $W_j(0)$ are balanced (see Definition 1), then
\[
\frac{dW(t)}{dt} = -A_W(t) \left( \nabla_W L^1(W(t)) \right).
\]
In the next section we will write this as a gradient flow with respect to a suitable Riemannian metric.

Finally, we recall the following result of Kawaguchi:

Theorem 5. [10] Theorem 2.3] Assume that $XX^T$ and $XY^T$ are of full rank with $d_y \leq d_x$ and that the matrix $YX^T(XX^T)^{-1}XY^T$ has $d_y$ distinct eigenvalues. Let $r$ be the minimum of the $d_y$. Then the loss function $L^N(W_1, \ldots, W_N)$ has the following properties.

1. It is non-convex and non-concave.
2. Every local minimum is a global minimum.
3. Every critical point that is not a global minimum is a saddle point.
4. If $W_{N-1} \cdots W_2$ has rank $r$ then the Hessian at any saddle point has at least one negative eigenvalue.

3. Riemannian gradient flows

Recall that in order to define a gradient flow, it is necessary to also specify the local geometry of the space. More precisely, suppose that a differentiable manifold $M$ is given, on which a smooth function $x \mapsto E(x) \in \mathbb{R}$ is defined for all $x \in M$. Then the differential $dE(x)$ of $E$ at the point $x$ is a co-tangent vector, i.e., a linear map from the tangent space $T_x M$ to $\mathbb{R}$. On the other hand, the derivative along any curve $t \mapsto \gamma(t) \in M$ is a tangent vector. If now $g_x$ denotes a Riemannian metric on $M$ at $x$, then it is possible to associate to the differential $dE(x)$ a unique tangent vector $\nabla E(x)$, called the gradient of $E$ at $x$, that satisfies
\[
dE(x)v := g_x(\nabla E(x), v) \text{ for all tangent vectors } v \in T_x M.
\]
It is the tangent vector $\nabla E(x)$ that enters in the definition of gradient flow $\dot{\gamma}(t) = -\nabla E(\gamma(t))$.

In this section, we are interested in minimizing the functional $L^N$ introduced in \((\ref{eq:fnl})\) over the family of all matrices $W_1, \ldots, W_N$. This can be accomplished by considering the long-time limit of the gradient flow of $L^N$. Alternatively, we can lump all matrices together in the product $W := W_N \cdots W_1$ and minimize the functional $L^1$ defined in \((\ref{eq:fnl1})\). It was shown in \((\ref{eq:descent})\) that the gradient descent for $L^N$, even though the functional
Proof. We split the proof into four steps. 

In particular, $\mathcal{M}_r$ is a manifold for $A$ to the power of $d_s \times d_s$ matrices, from which we inherit the structure of a differentiable manifold for $\mathcal{M}_r$. We denote by $T_{\mathcal{M}_r}(\mathcal{M}_r)$ the tangential space of $\mathcal{M}_r$ at the point $W \in \mathcal{M}_r$. We have

$$T_W(\mathcal{M}_r) := \{ \bar{WA} + BW : A \in \mathbb{R}^{d_s \times d_s}, B \in \mathbb{R}^{d_s \times d_s} \}$$

see [3] Proposition 4.1. Inspired by [3], we use the operator $A_W$ to define a Riemannian metric on $\mathcal{M}_r$.

**Lemma 6.** For any given $W \in \mathbb{R}^{d_s \times d_s}$ let $r$ be the rank of $W$, so that $W \in \mathcal{M}_r$. Let $N \geq 2$. Then the map $A_W : \mathbb{R}^{d_s \times d_s} \to \mathbb{R}^{d_s \times d_s}$ defined in (25) is a self-adjoint endomorphism. Its image is $T_W(\mathcal{M}_r)$ and its kernel is (consequently) the orthogonal complement $T_W(\mathcal{M}_r)^\perp$ of $T_W(\mathcal{M}_r)$. The restriction of $A_W$ to arguments $Z \in T_W(\mathcal{M}_r)$ defines a self-adjoint and positive definite endomorphism

$$\bar{A}_W : T_W(\mathcal{M}_r) \to T_W(\mathcal{M}_r).$$

In particular, $\bar{A}_W$ is invertible and the inverse $\bar{A}_W^{-1}$ is self-adjoint and positive definite as well.

Here the notions self-adjoint, positive definite, and orthogonal complement are understood with respect to the Frobenius scalar product, which we denote by $(\cdot, \cdot)_F$. Recall that $(A,B)_F = \text{tr}(AB^T)$.

**Proof.** We split the proof into four steps.

**Step 1.** It is clear that $A_W$ defines an endomorphism of $\mathbb{R}^{d_s \times d_s}$.

To see that it is self-adjoint, we calculate, for $Z_1, Z_2 \in \mathbb{R}^{d_s \times d_s}$,

$$\langle A_W(Z_1), Z_2 \rangle_F = \text{tr} \left( \sum_{j=1}^N (WW^T)_{\frac{N-j}{N-1}} Z_1(W^TW)_{\frac{j}{N}} Z_2^T \right) = \text{tr} \left( \sum_{j=1}^N Z_1(W^TW)_{\frac{j}{N}} Z_2^T (WW^T)_{\frac{N-j}{N-1}} \right)$$

$$= \text{tr} (Z_1 A_W(Z_2)^T) = \langle Z_1, A_W(Z_2) \rangle_F.$$

We conclude that $A_W$ is indeed self-adjoint.

**Step 2.** Next we show that the image of $A_W$ lies in $T_W(\mathcal{M}_r)$; see (27). Let $W = USV^T$ be a singular value decomposition of $W$ (thus $U$ and $V$ are orthogonal matrices of dimensions $d_u \times d_u$ and $d_x \times d_x$, respectively, and $S$ is a diagonal matrix of size $d_u \times d_u$ whose first $r$ diagonal entries are positive, with the remaining entries being equal to 0). For any index $j < N$ we can write

$$(WW^T)_{\frac{N-j}{N-1}} = U(SS^T)_{\frac{N-j}{N-1}} U^T = USV^T VST^T DU^T = WVS^T U^T D,$$

where $D$ is a $d_u \times d_u$ diagonal matrix whose non-zero entries are the corresponding non-zero entries of $SS^T$ to the power of $\frac{N-j}{N-1}$. Similarly, for any $j > 1$ we can write

$$(W^TW)^{\frac{j-1}{j}} = V(ST^S)^{\frac{j-1}{j}} V^T = V D S^T U^T USV^T = V D S^T U^T W,$$

where $D$ is a $d_x \times d_x$ diagonal matrix whose non-zero entries are the corresponding non-zero entries of $S^T S$ to the power of $\frac{j-1}{j}$. We observe that every term in the sum (25) is of the form $WA$ or of the form $BW$ for suitable $A \in \mathbb{R}^{d_s \times d_s}$ or $B \in \mathbb{R}^{d_s \times d_s}$. Hence $A_W(Z) \in T_W(\mathcal{M}_r)$ for any $Z \in \mathbb{R}^{d_s \times d_s}$. It follows that the restriction of $A_W$ to $T_W(\mathcal{M}_r)$ defines a self-adjoint endomorphism $\bar{A}_W : T_W(\mathcal{M}_r) \to T_W(\mathcal{M}_r)$.

**Step 3.** Next we show that it is positive definite. For $Z = WA + BW \in T_W(\mathcal{M}_r)$, we need to establish that $(A_W(Z), Z)_F > 0$ if $Z \neq 0$. We will first show that for all $j \in \{1, \ldots, N\}$

$$\text{tr} \left( (WW^T)^{\frac{N-j}{N-1}} Z(W^TW)^{\frac{j-1}{j}} Z^T \right) \geq 0.$$  \hspace{1cm} (28)

Let again $W = USV^T$ be a singular value decomposition of $W$ and note again that

$$(WW^T)^{\frac{N-j}{N-1}} = U(SS^T)^{\frac{N-j}{N-1}} U^T \quad \text{and} \quad (W^TW)^{\frac{j-1}{j}} = V(ST^S)^{\frac{j-1}{j}} V^T.$$
Let us also define $R := U^T Z V$. It follows that
\[
\text{tr} \left( (W W^T)^{\frac{N-1}{N}} Z (W^T W)^{\frac{N-1}{N}} Z^T \right) = \text{tr} \left( (S S^T)^{\frac{N-1}{N}} U^T Z V (S^T S)^{\frac{N-1}{N}} V^T Z U \right) = \text{tr} \left( (S S^T)^{\frac{N-1}{N}} R (S^T S)^{\frac{N-1}{N}} R^T \right).
\]

Let $S_x$ and $S_y$ be the $d_x \times d_x$ and $d_y \times d_y$ diagonal matrices, respectively, with diagonals given by the diagonal of $S$, extended by zero entries if necessary. Let $p := \frac{N}{N-1}$ and $q := \frac{N}{N+1}$. Then
\[
\text{tr} \left( (S S^T)^{\frac{N-1}{N}} R (S^T S)^{\frac{1}{N-1}} R^T \right) = \text{tr} \left( S_y^p R S_y^q R^T \right) = \text{tr} \left( S_y^p R S_y^q R^T \right) = \text{tr} \left( (S_y^p R S_y^q) (S_y^p R S_y^q)^T \right) \geq 0.
\]

Then (28) follows for all $j \in \{1, \ldots, N\}$ and hence $\langle A_W(Z), Z \rangle_F \geq 0$.

Suppose now that $\langle A_W(Z), Z \rangle_F = 0$. Then
\[
\text{tr} \left( (W W^T)^{\frac{N-1}{N}} Z (W^T W)^{\frac{N-1}{N}} Z^T \right) = 0
\]
for all $j \in \{1, \ldots, N\}$. In particular, for $j = 1$ and $j = N$, we obtain with the above notation that
\[
S_y^p R = 0 \quad \text{and} \quad R S_y^q = 0,
\]
hence $S_y R = 0$ and $R S_y = 0$. The condition $R S_y = 0$ implies that the first $r$ columns of $R$ are zero; the condition $S_y R = 0$ implies that the first $r$ rows of $R$ are zero. Now
\[
R = U^T Z V = U^T (W A + B W)V = U^T (U S V^T A + B U S V^T)V = S V^T A + U^T B U S.
\]

In the matrix $S V^T A$ all entries outside the first $r$ rows are zero; in the matrix $U^T B U S$ all entries outside the first $r$ columns are zero. Therefore $R$ cannot have any nonzero entries that are not in one of the first $r$ rows or the first $r$ columns. It follows that $R = 0$ and therefore also $Z = 0$.

**Step 4.** We have shown that $A_W$ is positive definite thus invertible, and that $A_W$ and $A_W^*$ both have image $T_W(M_r)$. It remains to prove that the kernel of $A_W$ is the orthogonal complement of $T_W(M_r)$. This follows from the fact that $A_W$ is self-adjoint together with the general fact that for any endomorphism $f$ of an Euclidian vector space, the kernel of $f$ is the orthogonal complement of the image of the adjoint of $f$.  

**Definition 7.** We introduce a Riemannian metric $g$ on the manifold $M_r$ (for $r \leq d_x, d_y$) by
\[
g_W(Z_1, Z_2) := \langle A_W^{-1}(Z_1), Z_2 \rangle_F \tag{29}
\]
for any $W \in M_r$ and for all tangent vectors $Z_1, Z_2 \in T_W(M_r)$.

By Lemma 6 the map $g_W$ is well defined and defines indeed a scalar product on $T_W(M_r)$. For any differentiable function $f : \mathbb{R}^{d_x \times d_x} \to \mathbb{R}$, any $W \in M_r \subset \mathbb{R}^{d_x \times d_x}$, and any $Z \in T_W(M_r)$, we have
\[
g_W(A_W(\nabla f(W)), Z) = \langle A_W^{-1}(A_W(\nabla f(W))), Z \rangle_F = \langle \nabla f(W), Z \rangle_F = Df(W)Z,
\]
where $Df$ denotes the differential of $f$ (which can be computed from the derivative with respect to $W$). Note here that by Lemma 6 the two quantities $A_W^{-1}(A_W(\nabla f(W)))$ and $\nabla f(W)$ differ only by an element in $T_W(M_r)^\perp$, which is perpendicular to $Z$ with respect to the Frobenius norm, as noticed above. This allows us to identify $A_W(\nabla f(W))$ with the gradient of $f$ with respect to the new metric $g$. We write
\[
A_W(\nabla f(W)) := \nabla g f(W). \tag{30}
\]

In particular, we have for all $Z \in T_W(M_r)$ that $g_W(\nabla g f(W), Z) = Df(W)(Z)$. Let now $r := \min\{d_0, \ldots, d_N\}$ and recall that, in the balanced case, the evolution of the product $W = W_N \cdots W_1$ is given by (26).

**Corollary 8.** Suppose that $W_1(t), \ldots, W_N(t)$ are solutions of the gradient flow (28) of $L^N$, with initial values $W_i(0)$ that are balanced; recall Definition 3. For $t \in \mathbb{R}$ define the product $W(t) := W_N(t) \cdots W_1(t)$. If $W(0)$ is contained in $M_r$ (i.e., has rank $r$), then $W(t) \in M_r$ for all $t$ and solves the gradient flow equation
\[
\dot{W} = -\nabla g L^1(W), \tag{31}
\]
where $\nabla g$ denotes the Riemannian gradient of $L^1$ with respect to the metric $g$ defined in (29).
Lemma 6 shows that the flow respects $\mathcal{M}_r$, which means that $W(t) \in \mathcal{M}_r$ for all $t \in \mathbb{R}$. The equation \((31)\) is a reformulation of \((29)\) with the particular choice of $g$ in \((29)\) as the metric.

**Proposition 9.** For $N = 2$ and $W \in \mathcal{M}_r$ the inverse operator $\bar{A}_W^{-1}: T_W(\mathcal{M}_r) \rightarrow T_W(\mathcal{M}_r)$ is given by

\[
\bar{A}_W^{-1}(Y) = \int_0^\infty e^{-t(WW^T)^{\frac{1}{2}}} Ye^{-t(WW^T)^{\frac{1}{2}}} dt.
\]

**Proof.** This can be shown like \([5, \text{Theorem VII.2.3}]\). It is easy to see that the integral converges and that the result lies in $T_W(\mathcal{M}_r)$. Now one just applies $\bar{A}_W$ to the r.h.s. of \((32)\) and uses the chain rule. \(\square\)

Proposition 9 enables us to evaluate for $N = 2$ and $W \in \mathcal{M}_r$ the scalar product $gw$ explicitly. We have

\[
gw(Z_1, Z_2) = \langle \bar{A}_W^{-1}(Z_1), Z_2 \rangle_F = \int_0^\infty \text{tr} \left( e^{-t(WW^T)^{\frac{1}{2}}} Z_1 e^{-t(WW^T)^{\frac{1}{2}}} Z_2^T \right) dt.
\]

**Remark 10.** Our Riemannian metric $g$ is (in the limit $N \to \infty$) similar to the Bogoliubov inner product of quantum statistical mechanics, which is defined on the manifold of positive definite matrices; see \([6]\).

4. Convergence of the gradient flow

In this section we will show that the gradient flow always converges to a critical point of $L^N$, also called an equilibrium point in the following, provided that $XX^T$ has full rank. We do not assume balancedness of the initial data. A similar statement was shown in \([7, \text{Proposition 1}]\) and similarly as in loc. cit., our proof is based on Lojasiewicz’s Theorem, but the technical exposition differs and we do not need the assumption $d_y \leq d_x$ made in \([7]\). Let us first recall Lojasiewicz’s Theorem; see \([13, 6, 4, 17]\).

**Theorem 11.** If $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is analytic and the curve $t \mapsto x(t) \in \mathbb{R}^n$, $t \in [0, \infty)$, is bounded and a solution of the gradient flow equation $\dot{x}(t) = -\nabla f(x(t))$, then $x(t)$ converges to a critical point of $f$ as $t \to \infty$.

**Theorem 12.** Assume $XX^T$ has full rank. Then the flows $W_i(t)$ defined by \((5)\) and $W(t)$ given by \((6)\) are defined for all $t \geq 0$ and $(W_1, \ldots, W_N)$ converges to a critical point of $L^N$ as $t \to \infty$.

**Proof.** We split the proof into four steps.

**Step 1.** We first show that the flow $W(t)$ given by \((6)\) remains bounded for all $t$. For this it is enough to show that if $\|W\|_F$ is large enough (i.e., $\|W\|_F \geq C$ for some constant $C$) then $\frac{d}{dt}\|W(t)\|_F^2 \leq 0$.

Let us first assume that the $W_j(0)$ are balanced. We observe that

\[
\frac{d}{dt}\|W\|_F^2 = 2\langle W, \dot{W} \rangle_F = -2\langle W, A_W(\nabla_W L(W)) \rangle_F = -2\langle W, A_W(XX^T - YY^T) \rangle_F.
\]

Therefore it is enough to show that $\langle W, A_W(XX^T - YY^T) \rangle_F \geq 0$ or, equivalently, that

\[
\langle A_W(W), XX^T \rangle_F \geq \langle A_W(W), YY^T \rangle_F
\]

if $\|W\|_F$ is large enough. We will show first that $\langle A_W(W), XX^T \rangle_F > 0$ for all $W \neq 0$. As before we write $W = USV^T$ for a singular value decomposition of $W$ and compute

\[
\langle A_W(W), XX^T \rangle_F = \langle W, A_W(XX^T) \rangle_F = \langle A_W(XX^T), W \rangle_F
\]

\[
= \text{tr} \left( \sum_{j=1}^N (W^T)^j WXX^T(W^T)^j W^T \right).
\]
Rearranging terms, we obtain

\[ \langle A_W(W), WXX^T \rangle_F = \sum_{j=1}^{N} \text{tr} \left( U(S S^T)^{\frac{N-j}{N}} U^T U S V^T X X^T V (S^T S)^{\frac{j-1}{N}} V^T V S^T U^T \right) \]

\[ = \sum_{j=1}^{N} \text{tr} \left( (S S^T)^{\frac{N-j}{N}} S V^T X X^T V (S^T S)^{\frac{j-1}{N}} S^T \right) \]

\[ = \sum_{j=1}^{N} \text{tr} \left( (S^T S)^{\frac{N-j}{N}} S^T (S S^T)^{\frac{j-1}{N}} S V^T X X^T V \right) \]

\[ = \sum_{j=1}^{N} \text{tr} \left( (S^T S)^{\frac{N-j}{N}} V^T X X^T V \right) > 0. \]

The last sum is positive because of the following lemma. Note that \( S^T S \) is non-zero, symmetric, and positive semidefinite, and \( V^T X X^T V \) is symmetric and positive definite since \( XX^T \) has full rank, by assumption.

**Lemma 13.** Let \( A, B \) be symmetric real-valued quadratic matrices of the same dimensions and assume that \( A \) is non-zero and positive semidefinite and that \( B \) is positive definite. Then \( \text{tr}(AB) > 0 \).

Before proving this lemma, we finish the proof of Theorem 12.

**Step 2.** The inequality \( 33 \) follows from a scaling argument. Let \( \alpha \in \mathbb{R} \) be non-negative. Then

\[ A_{\alpha W}(\alpha W) = \sum_{j=1}^{N} \alpha^{\frac{N-j}{N}} (W W^T)^{\frac{N-j}{N}} \cdot \alpha W \cdot \alpha^{\frac{j-1}{N}} (W^T W)^{\frac{j-1}{N}} = \alpha^{3-\frac{3}{N}} A_W(W). \]

It follows that

\[ \langle A_{\alpha W}(\alpha W), \alpha WXX^T \rangle_F = \alpha^{4-\frac{3}{N}} \langle A_W(W), WXX^T \rangle_F, \]

\[ \langle A_{\alpha W}(\alpha W), YX^T \rangle_F = \alpha^{3-\frac{3}{N}} \langle A_W(W), YX^T \rangle_F. \]

We proved in Step 1 that \( \langle A_W(W), WXX^T \rangle_F > 0 \) for all \( W \neq 0 \). We therefore conclude that for any \( W \in \mathbb{R}^{d_x \times d_x} \) with \( \|W\|_F = 1 \) there exists a sufficiently large positive \( \alpha \) such that

\[ \langle A_{\alpha W}(\alpha W), WXX^T \rangle_F \geq \langle A_{\alpha W}(\alpha W), YX^T \rangle_F. \]

Let now

\[ S^1 := \{ W \in \mathbb{R}^{d_x \times d_x} : \|W\|_F = 1 \} \]

and consider the map

\[ \xi : S^1 \to \mathbb{R}, ~ W \mapsto \min\{ \alpha : \alpha \geq 1, \langle A_{\alpha W}(\alpha W), \alpha WXX^T - YX^T \rangle_F \geq 0 \}. \]

By the reasoning above, this map is well-defined and continuous. Since \( S^1 \) is compact the positive number

\[ C := \max\{ \xi(W) : W \in S^1 \} \]

is finite.

It follows that if \( \|W(t)\|_F \geq C \) then \( \frac{d}{dt} \langle W(t) \rangle_F^2 \leq 0 \). Hence \( \|W(t)\|_F \) remains bounded for all \( t \).

**Step 3.** Now we drop the balancedness assumption. Then

\[ \frac{dW(t)}{dt} = -\sum_{j=1}^{N} (W(t)W(t)^T)^{\frac{N-j}{N}} \cdot \nabla W^T L^1(W(t)) \cdot (W(t)^T W(t))^{\frac{j-1}{N}} + R(t), \]

where \( R \) depends on the \( W_j \) and satisfies

\[ \|R\|_F \leq C_1 \|W\|_F^3 \cdot \frac{1}{N} + C_2 \]

for suitable positive constants \( C_1, C_2 \); see Lemma 2 (5). As before, we obtain

\[ \frac{d}{dt} \|W\|_F^2 = 2 \langle W, \dot{W} \rangle_F = 2 \langle W, -A_W(\nabla W^T L^1(W)) + R \rangle_F = -2 \langle W, A_W(WXX^T - YX^T) - R \rangle_F, \]
and so it is sufficient to show that, whenever \( \|W\|_F \) is large enough, we have
\[
\langle AW(W), WX^T X^T \rangle_F \geq \langle AW(W), YX^T \rangle_F + \langle W, R \rangle_F
\]

Multiplying \( W \) by \( \alpha \) we get a factor \( \alpha^{4-\frac{2}{N}} \) on the left-hand side. On the other hand, it holds
\[
|\langle W, R \rangle_F| \leq C_1 \|W\|_F^{4-\frac{2}{N}} + C_2 \|W\|_F
\]
and \( 4 - \frac{2}{N} < 4 - \frac{2}{N} \). Thus we can argue analogously to the reasoning above.

**Step 4.** The fact that all the \( \|W_i\|_F \) are bounded follows from estimate (9). This ensures the existence of solutions \( W_i(t) \) (and hence \( W(t) \)) for all \( t \geq 0 \); cf. also [11, Section 4.2.III]. The convergence of \( (W_1, \ldots, W_N) \) to an equilibrium point (i.e., a critical point of \( L^N \)) now follows from Lojasiewicz’s Theorem 11. □

**Proof of Lemma [13]** We use the spectral theorem: Since \( A \) is symmetric and positive semidefinite, there exists eigenvalues \( \lambda_i \geq 0 \) with corresponding eigenvectors \( v_i \neq 0 \) such that
\[
A = \sum_i \lambda_i v_i \otimes v_i.
\]
Since \( A \) is non-zero, there exists at least one index \( j \) with \( \lambda_j > 0 \). Then
\[
\text{tr}(AB) = \sum_i \lambda_i \text{tr}((v_i \otimes v_i)B) \geq \lambda_j v_j^T B v_j.
\]
Since \( B \) is positive definite, we have that \( v^T B v > 0 \) for all \( v \neq 0 \), and thus \( \text{tr}(AB) > 0 \). □

5. Linear Autoencoders with one hidden layer

In this section we consider linear autoencoders with one hidden layer, i.e., we assume \( Y = X \) and \( N = 2 \).

5.1. The symmetric case. Here we consider the optimization problem [11] with \( N = 2 \) and the additional constraints that \( Y = X \) and \( W_2 = W_1^T \). For \( V := W_2 = W_1 \in \mathbb{R}^{d \times r} \) (where we write \( d \) for \( d_x = d_y \) and \( r \) for \( d_1 \)), let
\[
E(V) = L^2(V^T, V) = \frac{1}{2} \|X - VV^T X\|_F^2.
\]

We consider the gradient flow:
\[
\dot{V} = -\nabla E(V), \quad V(0) = V_0,
\]
where we assume that \( V_0^T V_0 = I_r \). Computing the gradient of \( E \) gives
\[
\nabla E(V) = -(I_d - VV^T)XX^T V - X^T(I_d - VV^T)V.
\]

Thus the gradient flow for \( V \) is given by
\[
\dot{V} = (I_d - VV^T)XX^TV + XX^T(V(I_d - VV^T)V), \quad V(0) = V_0, \quad V_0^T V_0 = I_r.
\]

This can be analyzed using results by Helmke, Moore, and Yan on Oja’s flow [18].

**Theorem 14.**
(1) The flow (36) has a unique solution on the intervall \([0, \infty)\).
(2) \( V(t) V(t) = I_r \) for all \( t \geq 0 \).
(3) The limit \( V = \lim_{t \to \infty} V(t) \) exists and it is an equilibrium.
(4) The convergence is exponentially: There are positive constants \( c_1, c_2 \) such that
\[
\|V(t) - V\|_F \leq c_1 e^{-c_2 t}
\]
for all \( t \geq 0 \).
(5) The equilibrium points of the flow (36) are precisely the matrices of the form
\[
V = (v_1 \cdots v_r) Q,
\]
where \( v_1, \ldots, v_r \) are orthonormal eigenvectors of \( XX^T \) and \( Q \) is an orthogonal \( r \times r \)-matrix.
Proof. In [18] it is shown that Oja’s flow given by

\[ \dot{V} = (I_d - VV^T)XX^TV \]

satisfies all the claims in the proposition provided that \( V(0)^TV(0) = I_r \). In particular, by [18] Corollary 2.1, all \( V(t) \) in any solution of Oja’s flow with \( V(0)^TV(0) = I_r \) fulfill \( V(t)^TV(t) = I_r \). It follows that under the initial condition \( V(0)^TV(0) = I_r \), the flow (36) is identical to Oja’s flow because the term \( XX^T(I_d - VV^T)V \) then vanishes for all \( t \) if \( V \) is a solution to Oja’s flow.

Hence, (2) follows from [18] Corollary 2.1. In [18] Theorem 2.1 an existence and uniqueness result on [18, Corollary 2.1]. □

**Remark 15.** Choosing \( v_1, \ldots, v_r \) orthonormal eigenvectors corresponding to the largest \( r \) eigenvalues of \( XX^T \), we obtain (for varying \( Q \)) precisely the possible solutions for the matrix \( V \) in the PCA-problem.

In order to make this more precise and to see this claim, we recall the PCA-Theorem, cf. [14]. Given: \( x_1, \ldots, x_m \in \mathbb{R}^d \) and \( 1 \leq r \leq d \), we consider the following problem: Find \( v_1, \ldots, v_r \in \mathbb{R}^d \) orthonormal and \( h_1, \ldots, h_m \in \mathbb{R}^r \) such that

\[ \mathcal{L}(V; h_1, \ldots, h_m) := \frac{1}{m} \sum_i \|x_i - Vh_i\|^2 \]  

is minimal. (Here \( V = (v_1 | \ldots | v_r) \in \mathbb{R}^{d \times r} \).

**Theorem 16 (PCA-Theorem [14]).** A minimizer of (37) is obtained by choosing \( v_1, \ldots, v_r \) as orthonormal eigenvectors corresponding to the \( r \) largest eigenvalues of \( \sum_i x_ix_i^T = XX^T \) and \( h_i = V^Tx_i \).

The other possible solutions for \( V \) are of the form \( V = (v_1 | \ldots | v_r) Q \), where \( v_1, \ldots, v_r \) are chosen as above and \( Q \) is an orthogonal \( r \times r \)-matrix. Again \( h_i = V^Tx_i \).

Let \( \lambda_1 \geq \ldots \geq \lambda_d \) be the eigenvalues of \( XX^T \) and let \( v_1, \ldots, v_d \) be corresponding orthonormal eigenvectors.

**Theorem 17.** Assume that \( XX^T \) has full rank and that \( \lambda_i > \lambda_{i+1} \). Then \( \lim_{t \to \infty} V(t) = (v_1 | \ldots | v_r) Q \) for some orthogonal \( Q \) if and only if \( V(t) \) has rank \( r \).

Proof. This follows from [18] Theorem 5.1] (where an analogous statement for Oja’s flow is made) together with [18] Corollary 2.1. □

**Corollary 18.** Under the assumptions of Theorem 17, for almost all initial conditions (w.r.t. the Lebesgue measure), the flow converges to an optimal equilibrium, i.e. one of the form \( V = (v_1 | \ldots | v_r) Q \) in the notation of Theorem 17.

Proof. This follows from Theorem [17] cf. also the analogous [18] Corollary 5.1. □

In Section 6 we extend this result to autoencoders with \( N > 2 \) layers using a more abstract approach. The following theorem shows that the optimal equilibria are the only stable equilibria:

**Theorem 19.** Assume \( V = (v_1 | \ldots | v_r) Q \), where the orthonormal eigenvectors \( v_1, \ldots, v_r \) are not eigenvectors corresponding to the largest \( r \) eigenvalues of \( XX^T \). Then in any neighborhood of \( V \) there is a matrix \( \tilde{V} \) with \( E(\tilde{V}) < E(V) \) (and \( \tilde{V}^TV = I_r \)).

Proof. Let \( v_i \) be one of the eigenvectors \( v_1, \ldots, v_r \) whose eigenvalue does not belong to the \( r \) largest eigenvalues of \( XX^T \). Let \( v \) be an eigenvector of \( XX^T \) of unit length which is orthogonal to the eigenvectors \( v_1, \ldots, v_r \) and whose eigenvalue belongs to the \( r \) largest eigenvalues of \( XX^T \). Now for any \( \varepsilon \in [0, 1] \) consider \( v_i(\varepsilon) := \varepsilon v + \sqrt{1 - \varepsilon^2}v_i \). Then \( V(\varepsilon) := (v_1 | \ldots | v_i(\varepsilon) | \ldots | v_r) Q \) satisfies \( E(V(\varepsilon)) < E(V) \) for \( \varepsilon \in (0, 1] \) and \( V(\varepsilon)^TV(\varepsilon) = I_r \). From this the claim follows. □
5.2. The non-symmetric case. Here we consider the optimization problem \((1)\) with \(N = 2\) and the additional constraint that \(Y = X\), but we do not assume that \(W_2 = W_1^T\). We also assume balanced starting conditions, i.e., \(W_2(0)^T W_2(0) = W_1(0) W_1(0)^T\). We write again \(d\) for \(d_x = d_y\) and \(r\) for \(d_1\).

The equations for the flow here are:

\[
\begin{align*}
\dot{W}_1 & = -W_2^T W_2 W_1 X X^T + W_2^T X X^T, \\
\dot{W}_2 & = -W_2 W_1 X X^T W_1^T + X X^T W_1^T.
\end{align*}
\]  

(38)

Remark 20. With the notations

\[
V = \begin{pmatrix} W_1^T \\ W_2 \end{pmatrix} \in \mathbb{R}^{2d \times r} \text{ and } C = X X^T \in \mathbb{R}^{d \times d}
\]

and assuming that \(C = X X^T\) has full rank, the flow (38) can be written as the following Riccati-type-like ODE.

\[
\dot{V} = \begin{pmatrix} I_{2d} + \begin{pmatrix} -C & 0 \\ 0 & 0 \end{pmatrix} & V V^T \begin{pmatrix} 0 & 0 \\ C^{-1} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & -I_d \end{pmatrix} V V^T \begin{pmatrix} 0 & I_d \\ 0 & 0 \end{pmatrix} \end{pmatrix} \begin{pmatrix} 0 & C \\ C & 0 \end{pmatrix} V.
\]  

(39)

Next we analyze the equilibrium points of the flow (38) and of the product \(W = W_2 W_1\) again assuming balanced initial conditions. We begin by exploring the equilibrium points of the flow (38) by setting the expressions in (38) equal to zero:

\[
\begin{align*}
-W_2^T W_2 W_1 X X^T + W_2^T X X^T &= 0, \\
-W_2 W_1 X X^T W_1^T + X X^T W_1^T &= 0.
\end{align*}
\]  

(40)

If \(W_2 \in \mathbb{R}^{d \times r}\) is the zero matrix then (since \(X X^T\) has full rank) it follows that (40) is solved if and only if \(W_1\) is the \(r \times d\) zero-matrix, hence \(W\) is the \(d \times d\) zero-matrix. The following lemma characterizes the non-trivial solutions.

Lemma 21. The balanced nonzero-solutions (i.e. solutions with \(W_2 \neq 0\)) of (40) are precisely the matrices of the form

\[
\begin{align*}
W_2 &= U V^T, \\
W_1 &= W_2^T = V U^T, \\
W &= W_2 W_1 = U U^T,
\end{align*}
\]

where \(U \in \mathbb{R}^{d \times k}\) for some \(k \leq r\) and where the columns of \(U\) are orthonormal eigenvectors of \(X X^T\) and \(V \in \mathbb{R}^{r \times k}\) has orthonormal columns.

In particular, the equilibrium points for \(W = W_2 W_1\) are precisely the matrices of the form

\[
W = \sum_{j=1}^{k} u_j u_j^T,
\]

where \(k \in \{0, \ldots, r\}\) and \(u_1, \ldots, u_k\) (the columns of \(U\) above) are orthonormal eigenvectors of \(X X^T\).

Proof. Since \(W_2 \neq 0\), the rank \(k\) of \(W_2\) is at least 1. The balancedness condition \(W_2^T W_2 = W_1 W_1^T\) implies that \(W_1\) and \(W_2\) have the same singular values. Since \(X X^T\) has full rank, the first equation of (40) yields \(W_2^T = W_2^T W_2 W_1\). Again due to balancedness, this shows that \(W_2^T = W_1 W_1^T W_2\). It follows that all positive singular values of \(W_1\) and of \(W_2\) are equal to 1 and that \(W_2 = W_1^T\). The second equation of (40) thus gives the equation

\[
(I_d - W_2 W_2^T) X X^T W_2 = 0.
\]  

(41)

(The equilibrium points of full rank \(r\) could now be obtained using [18], Proposition 4.1] again, but we are interested in all solutions here.) Since the positive singular values of \(W_2\) are all equal to 1, it follows that we can write

\[
W_2 W_2^T = \sum_{i=1}^{k} u_i u_i^T,
\]
where the \( u_i \) are orthonormal. We extend the system \( u_1, \ldots, u_k \) to an orthonormal basis \( u_1, \ldots, u_d \) of \( \mathbb{R}^d \). From (41) we obtain \((I_d - W_2 W_2^T)XX^T W_2 W_2^T = 0\) and hence
\[
\sum_{j=k+1}^d u_j u_j^T XX^T \sum_{i=1}^k u_i u_i^T = 0.
\]
Hence
\[
\sum_{j=k+1}^d \sum_{i=1}^k (u_j^T XX^T u_i) u_j u_i^T = 0.
\]
It follows that for all \( j \in \{k+1, \ldots, d\} \) and for all \( i \in \{1, \ldots, k\} \) we have \( u_j^T XX^T u_i = 0 \). This in turn implies that \( XX^T \) maps the span of \( u_1, \ldots, u_k \) into itself and also maps the span of \( u_{k+1}, \ldots, u_d \) into itself. This implies that we can choose \( u_1, \ldots, u_d \) as orthonormal eigenvectors of \( XX^T \). Thus we can indeed write the (reduced) singular value decomposition of \( W_2 \) as \( W_2 = UV^T \), where the columns \( u_1, \ldots, u_k \) of \( U \) are orthonormal eigenvectors of \( XX^T \) and where \( V \) is as in the statement of the lemma. Since \( W_1 = W_2^T \) and \( W = W_2 W_1 \), it follows that \( W_1 = VU^T \) and \( W = UVT \) as claimed. Conversely, if \( U, V, W_1, W_2 \) are as in the statement of the lemma, one easily checks that (40) is fulfilled. This ends the proof. \( \square \)

**Corollary 22.** Consider a linear autoencoder with one hidden layer of size \( r \) with balanced initial conditions and assume that \( XX^T \) has eigenvalues \( \lambda_1 \geq \ldots \geq \lambda_d > 0 \) and corresponding orthonormal eigenvectors \( u_1, \ldots, u_d \).

1. The flow \( W(t) \) always converges to an equilibrium point of the form \( W = \sum_{j \in J_W} u_j u_j^T \), where \( J_W \) is a (possibly empty) subset of \( \{1, \ldots, d\} \) of at most \( r \) elements.
2. The flow \( W(t) \) converges to \( UV^T \), where the columns of \( U \) are the \( u_j \), \( j \in J_W \), and \( V \in \mathbb{R}^{r \times k} \) has orthonormal columns \( (k = |J_W|) \). Furthermore \( W_1(t) \) converges to \( W_2^T \).
3. If \( L(W(0)) < \frac{1}{1} \sum_{i=r+1}^d \lambda_i \) then \( W(t) \) converges to the optimal equilibrium \( W = \sum_{j=1}^r u_j u_j^T \).
4. If \( \lambda_r > \lambda_{r+1} \), then there is an open neighbourhood of the optimal equilibrium point in which we have convergence of the flow \( W(t) \) to the optimal equilibrium point.

**Proof.** The first and the second point follow from Lemma 21 together with Theorem 12 (Note that if \( (W_1, W_2) \) is an equilibrium point to which the flow converges then \( W_1, W_2 \) are balanced since we assume that the flow has balanced initial conditions.) To prove the third point, note that the loss of an equilibrium point \( W = \sum_{j \in J_W} u_j u_j^T \) is given by \( L(W) = \frac{1}{2} \sum_{i \in I_W} \lambda_i \), where \( I_W = \{1, \ldots, d\} \setminus J_W \). This sum is minimal for \( J_W = \{1, \ldots, r\} \). Among the remaining possible \( J_W \), the value of \( L(W) \) is minimal for \( J_W = \{1, \ldots, r\} \setminus \{r+1\} \), i.e. \( I_W = \{r, \ldots, d\} \setminus \{r+1\} \). Since the value of \( L(W(t)) \) monotonically decreases as \( t \) increases (as follows e.g. from equation (31)), the claim now follows from the first point. The last point follows from the third point. \( \square \)

The following result is an analogue to Theorem 19.

**Theorem 23.** If \( k \leq r \) and \( u_1, \ldots, u_k \) are orthonormal eigenvectors of \( XX^T \) which do not form a system of eigenvectors to the \( r \) largest eigenvalues of \( XX^T \) (in particular for \( k < r \)), in any neighborhood of the equilibrium point \( W = \sum_{j=1}^k u_j u_j^T \) there is some \( W \) of rank at most \( r \) for which \( L(W) < L(W) \). In particular, the equilibrium in \( W \) is non-stable.

**Proof.** If \( k < r \) and \( W = \sum_{j=1}^k u_j u_j^T \) for orthonormal eigenvectors \( u_j \) of \( XX^T \) then for any additional eigenvector \( u_{k+1} \) orthonormal to the \( u_j \) and for any \( \varepsilon > 0 \), we can choose \( W = W + \varepsilon u_{k+1} u_{k+1}^T \) to obtain \( L(W) < L(W) \). Let now \( k = r \). This case can be treated analogously to the proof of Theorem 19; let \( u_1 \) be one of the eigenvectors \( u_1, \ldots, u_r \), whose eigenvalue does not belong to the \( r \) largest eigenvalues of \( XX^T \). Let \( v \) be an eigenvector of \( XX^T \) of unit length which is orthogonal to the eigenvectors \( u_1, \ldots, u_r \) and whose eigenvalue belongs to the \( r \) largest eigenvalues of \( XX^T \). Now for any \( \varepsilon \in [0, 1] \) consider \( u_1(\varepsilon) := \varepsilon v + \sqrt{1 - \varepsilon^2} u_1 \). Then \( W(\varepsilon) := u_1(\varepsilon) u_1(\varepsilon)^T + \sum_{j=1, j \neq 1} u_j u_j^T \) satisfies \( L(W(\varepsilon)) < L(W) \) for \( \varepsilon \in [0, 1] \). From this the claim follows. \( \square \)
6. Avoiding saddle points

In Section 4 we have proven convergence of the gradient flow \([\mathbf{4}]\) and Riemannian gradient flow \([\mathbf{31}]\) to critical points of \(L^N\) and \(L^1\) restricted to \(\mathcal{M}_r\), respectively. Since we will remain in a saddle point forever if the initial point is a saddle point, the best we can hope for is convergence to global optima for almost all initial points (as in Corollary \([\mathbf{18}]\) for the particular autoencoder case with \(N = 2\)). We will indeed establish such a result for \(L^1\) restricted to \(\mathcal{M}_r\) in the autoencoder case for general number \(N \geq 2\) of layers for balanced initial conditions by showing a general result on the avoidance of saddle points by extending the main result of \([\mathbf{12}]\) from gradient descent to gradient flows. A crucial ingredient is the notion of a strict saddle point. The application of the general abstract result to our scenario then requires to show that all saddle points of the functional \(L^1\) restricted to \(\mathcal{M}_r\) are strict.

6.1. Strict saddle points. We start with the definition of a strict saddle point of a function on Euclidean space \(\mathbb{R}^d\).

**Definition 24.** Let \(f : \Omega \to \mathbb{R}\) be a twice continuously differentiable function on an open domain \(\Omega \subset \mathbb{R}^d\). A critical point \(x_0 \in \Omega\) is called a strict saddle point if the Hessian \(H_f(x_0)\) has a negative eigenvalue.

Intuitively, the function \(f\) possesses a direction of descent at a strict saddle point. Note that our definition also includes local maxima, which does not pose problems for our purposes.

Let us extend the notion of strict saddle points to functions on Riemannian manifolds \((\mathcal{M}, g)\). To this end, we first introduce the Riemannian Hessian of a \(C^2\)-function \(f\) on \(\mathcal{M}\). Denoting by \(\nabla\) be the Riemannian connection (Levi-Civita connection) on \((\mathcal{M}, g)\) the Riemannian Hessian of \(f\) at \(x \in \mathcal{M}\) is the linear mapping \(\text{Hess} f(x) : T_x \mathcal{M} \to \mathcal{M}\) defined by

\[
\text{Hess} f(x)[\xi] := \nabla_x \nabla^g f.
\]

Of course, if \((\mathcal{M}, g)\) is Euclidean, then this definition can be identified with the standard definition of the Hessian. Moreover, if \(x \in \mathcal{M}\) is a critical point of \(f\), i.e., \(\nabla^g f(x) = 0\), then the Riemannian Hess \(\text{Hess} f(x)\) is independent of the choice of the connection. Below, we will need the following chain type rule for curves \(\gamma\) on \(\mathcal{M}\), see e.g. \([\mathbf{15}]\) Eq. (3.19)),

\[
\frac{d^2}{dt^2} f(\gamma(t)) = g(\dot{\gamma}(t), \text{Hess}^g f(\gamma(t)) \dot{\gamma}(t)) + g\left( \frac{D}{dt} \dot{\gamma}(t), \nabla^g f(\gamma(t)) \right),
\]

where \(\frac{D}{dt} \dot{\gamma}(t)\) is related to the Riemannian connection that is used to define the Hessian, see \([\mathbf{2}]\) Section 5.4]. We refer to \([\mathbf{2}]\) for more details on the Riemannian Hessian.

**Definition 25.** Let \((\mathcal{M}, g)\) be a Riemannian manifold with Levi-Civita connection \(\nabla^g\) and let \(f : \mathcal{M} \to \mathbb{R}\) be a twice continuously differentiable. A critical point \(x_0 \in \mathcal{M}\), i.e., \(\nabla^g f(x_0) = 0\) is called a strict saddle point if \(\text{Hess} f(x)\) has a negative eigenvalue. We denote the set of all strict saddles of \(f\) by \(\mathcal{X} = \mathcal{X}(f)\). We say that \(f\) has the strict saddle point property, if all critical points of \(f\) that are not local minima are strict saddle points.

Note that our definition of strict saddle points includes local maxima, which is fine for our purposes.

6.2. Flows avoid strict saddle points almost surely. We now prove a general result that gradient flows on a Riemannian manifold \((\mathcal{M}, g)\) for functions with the strict saddle point property avoid saddle point for almost all initial values. This result extends the main result of \([\mathbf{12}]\) from time discrete systems to continuous flows and should be of independent interest.

For a continuously differentiable function \(L : \mathcal{M} \to \mathbb{R}\), we consider the Riemannian gradient flow

\[
\frac{d}{dt} \phi(t) = -\nabla^g L(\phi(t)), \quad \phi(0) = x_0 \in \mathcal{M},
\]

where \(\nabla^g\) denotes the Riemannian gradient. When emphasizing the dependence on \(x_0\), we write

\[
\psi_\phi(x_0) = \phi(t),
\]

where \(\phi(t)\) is the solution to \([\mathbf{43}]\) with initial condition \(x_0\).

Sets of measure zero on \(\mathcal{M}\) (as used in the next theorem) can be defined using push forwards of the Lebesgue measure on charts of the manifold \(\mathcal{M}\).
Theorem 26. Let \( L : M \to \mathbb{R} \) be a twice continuously differentiable function on a second countable Riemannian manifold \( (M, g) \). If \( L \) has the strict saddle point property, then the set
\[
W_L := \{ x_0 \in M : \lim_{t \to \infty} \psi(x_0) \in X = X(L) \}
\]
of initial points such that the corresponding flow converges to (strict) saddles has measure zero.

The proof of this relies on the following result for iteration maps (e.g., gradient descent iterations) shown in [12].

Theorem 27. Let \( h : M \to \mathbb{R} \) be a continuously differentiable function on a second countable differentiable finite-dimensional manifold such that \( \det(Dh(x)) \neq 0 \) for all \( x \in M \) (in particular, \( h \) is a local \( C^1 \) diffeomorphism). Let
\[
A_h^* = \{ x \in M : h(x) = x, \max_j |\lambda_j(Dh(x))| > 1 \},
\]
where \( \lambda_j(Dh(x)) \) denote the eigenvalues of \( Dh(x) \), and consider sequences with initial point \( x_0 \in M \), \( x_k = h(x_{k-1}) \), \( k \in \mathbb{N} \). Then the set \( \{ x_0 \in M : \lim_{k \to \infty} x_k \in A_h^* \} \) has measure zero.

Proof of Theorem 27. For a fixed \( T > 0 \), we introduce the function \( h : M \to \mathbb{R} \), \( h(x_0) = \phi_T(x_0) \). Since \( L \) is twice continuously differentiable, it follows that \( h \) is continuously differentiable. By the property \( \phi_{T+s}(x_0) = \phi_T(\phi_s(x_0)) \), it holds that the sequence \( x_k = \phi_{kT}(x_0) \), \( k \in \mathbb{N} \) satisfies \( x_k = h(x_{k-1}) \) and \( \lim_{k \to \infty} x_k \in X \) implies \( \lim_{k \to \infty} x_k \in X \), so that with the notation of Theorem 27, we have
\[
W_L \subset \{ x_0 \in M : \lim_{k \to \infty} x_k \in X \}.
\]

Therefore, in order to apply Theorem 27, we need to show that \( X \subset A_h^* \) and that \( \det(Dh(x)) \neq 0 \) for all \( x \in M \). To this end, we use that \( h \) is related to \( L \) via the gradient flow equation (43) and that therefore, the differential of \( h \) is related to the Riemannian Hessian of \( L \), see e.g., [16, Lemma 4.5],
\[
Dh(x) = \exp(-\text{Hess } L(x)).
\]
This relation clearly implies that \( Dh(x) \) is nonsingular for all \( x \in M \) (which is related to the fact, that \( h(-1) = \phi_{-T}(x) \), i.e., the gradient flow is reversible). Moreover, if \( x_0 \in M \) is a saddle point, then by the strict saddle property, the Hessian \( \text{Hess } f(x_0) \) has a strictly negative eigenvalue, which implies by (45) that the largest eigenvalue of \( Dh(x_0) \) is larger than 1 so that \( X \subset A_h^* \). This concludes the proof. \( \square \)

Remark 28. The proof of the main ingredient of Theorem 26 uses the center and stable manifold theorem, see, e.g., [16, Chapter, Theorem III.7]. If the absolute eigenvalues of \( Dh(x) \) are all different from 1, i.e., if all eigenvalues of the Hessian \( \text{Hess } f(x) \) are different from 0 at saddle points \( x \), then slightly stronger conclusions may be drawn, including the speed at which the flow moves away from saddle points. We will not elaborate on this point here.

6.3. The strict saddle point property for \( L^1 \) on \( M_c \). In this section we establish the strict saddle point property of \( L^1 \) on \( M_c \), in the autoencoder case \( Y = X \) by showing that the Riemannian Hessian \( L^1 \) at all critical points that are not a global minimizer has a strictly negative eigenvalue.

We assume that \( Y = X \) and that \( XX^T \in \mathbb{R}^{d \times d} \) has full rank. Let \( r \leq d \) and let \( g \) be an arbitrary Riemannian metric on the manifold \( M_c \) of all \( d \times d \) matrices of rank \( r \), for example it could be the metric induced by the standard metric on \( \mathbb{R}^{d \times d} \) or the metric \( g \) introduced in section 5 for some number of layers \( N \).

The next statement is similar in spirit to Kawaguchi’s result, Theorem 5 but more precise.

Proposition 29. (1) The critical points of \( L^1 \) on \( M_c \) are precisely the matrices of the form
\[
W = \sum_{j=1}^r u_j u_j^T,
\]
where \( u_1, \ldots, u_r \) are orthonormal eigenvectors of \( XX^T \).
(2) If $W$ is as above and $\lambda_j$ denotes the eigenvalue of $XX^T$ corresponding to $u_j$ then

$$L^1(W) = \frac{1}{2} \left( \text{tr}(XX^T) - \sum_{j=1}^{r} \lambda_j \right).$$

In particular, $W$ is a global minimizer of $L^1$ on $\mathcal{M}_r$ if and only if $u_1, \ldots, u_r$ are orthonormal eigenvectors corresponding to the largest $r$ eigenvalues of $XX^T$.

Proof. Recall that for $Y = X$ the gradient $\nabla L^1(W)$ is given by $\nabla L^1(W) = WXX^T - XX^T$. A matrix $W \in \mathcal{M}_r$ is a critical point of $L^1$ on $\mathcal{M}_r$ if and only if $\nabla L^1(W)$ is perpendicular to the tangent space $T_W(\mathcal{M}_r)$ of $\mathcal{M}_r$ in $W$. Recall that $T_W(\mathcal{M}_r)$ consists of all matrices in the set $\{WA + BW, \ A, B \in \mathbb{R}^{d \times d}\}$. Thus $W \in \mathcal{M}_r$ is a critical point if and only if $\langle \nabla L^1(W), W \rangle = 0$ and $\langle \nabla L^1(W), B \rangle = 0$ for all $A, B \in \mathbb{R}^{d \times d}$. This is equivalent to $\langle W^T \nabla L^1(W), A \rangle = 0$ and $\langle \nabla L^1(W)W^T, B \rangle = 0$ for all $A, B \in \mathbb{R}^{d \times d}$ and this in turn is equivalent to $W^T \nabla L^1(W) = 0$ and $\nabla L^1(W)W^T = 0$. Hence $W \in \mathcal{M}_r$ is a critical point of $L^1$ on $\mathcal{M}_r$ if and only if

$$W^T(W - I_d)XX^T = 0,$$

$$(W - I_d)XX^TW^T = 0. \quad (46)$$

The remainder of the proof essentially follows the reasoning in the proof of Lemma 21, but we include it here for completeness. Since $XX^T$ has full rank, the first equation of (46) is equivalent to $W^TW = W^T$. The second equation of (46) is equivalent to

$$WXX^T(W^T - I_d) = 0.$$

Together with $W^TW = W^T$ this implies that

$$W^TXX^T(I_d - W^TW) = 0.$$

Since $W^TW = W^T$, all singular values of $W$ and of $W^T$ are 0 or 1, and all eigenvalues of $W^TW$ are 0 or 1. Thus we can write $W^TW = \sum_{i=1}^{r} u_iu_i^T$ for suitable orthonormal vectors $u_1, \ldots, u_r$. We want to show that we can choose orthonormal eigenvectors of $XX^T$ for $u_1, \ldots, u_r$. Extend $u_1, \ldots, u_r$ to an orthonormal basis $u_1, \ldots, u_d$ of $\mathbb{R}^d$. Then the relation $W^TXX^T(I_d - W^TW) = 0$ can be written as

$$\sum_{i=1}^{r} u_iu_i^TXX^T \sum_{j=r+1}^{d} u_ju_j^T = 0.$$

Hence

$$\sum_{i=1}^{r} \sum_{j=r+1}^{d} (u_i^TXX^T u_j) u_i u_j^T = 0.$$

It follows that for all $i \in \{1, \ldots, r\}$ and for all $j \in \{r + 1, \ldots, d\}$ we have $u_i^TXX^T u_j = 0$, since the matrices $u_iu_j^T$ are orthonormal with respect to the Frobenius scalar product, in particular they are linearly independent. This in turn implies that $XX^T$ maps the span of $u_1, \ldots, u_r$ into itself and also maps the span of $u_{r+1}, \ldots, u_d$ into itself. This implies that we can choose $u_1, \ldots, u_d$ as orthonormal eigenvectors of $XX^T$. It follows that $W$ is indeed of the form

$$W = \sum_{j=1}^{r} u_j u_j^T,$$

where $u_1, \ldots, u_r$ are orthonormal eigenvectors of $XX^T$. Conversely, any matrix $W$ of this form obviously satisfies the equations in (46).

The proof of the second statement of the proposition follows by straightforward calculation. \qed

Proposition 30. The function $L^1$ on $\mathcal{M}_r$ satisfies the strict saddle point property. More precisely, all critical points of $L^1$ on $\mathcal{M}_r$ except for the global minimizers are strict saddle points.
Proof. By Proposition 23 it is enough to show that the Riemannian Hessian of $L^1$ has a negative eigenvalue at any point of the form

$$W = \sum_{j=1}^{r} u_j u_j^T,$$

where $u_1, \ldots, u_r$ are orthonormal eigenvectors of $XX^T$ and where the eigenvalue of at least one of the eigenvectors $u_1, \ldots, u_r$ is not among the $r$ largest eigenvalues of $XX^T$. Proceeding similarly as in the proofs of Theorems 19 and 23, given such a point $W$, let $u_i$ be one of the eigenvectors $u_1, \ldots, u_r$ whose eigenvalue does not belong to the $r$ largest eigenvalues of $XX^T$. Let $u_0$ be an eigenvector of $XX^T$ of unit length which is orthogonal to the eigenvectors $u_1, \ldots, u_r$ and whose eigenvalue belongs to the $r$ largest eigenvalues of $XX^T$. For $t \in (-1, 1)$ let $u_i(t) := tu_i + \sqrt{1-t^2}u_i$.

Now consider the curve $\gamma : (-1, 1) \to M_r$ given by $\gamma(t) = u_i(t)u_i(t)^T + \sum_{j=1, j \neq i}^{r} u_j u_j^T$. Obviously we have $\gamma(0) = W$. We claim that it is enough to show that

$$\left. \frac{d^2}{dt^2} L^1(\gamma(t)) \right|_{t=0} < 0.$$

Indeed, by [12] it holds (for any Riemannian metric $g$) that

$$\frac{d^2}{dt^2} L^1(\gamma(t)) = g(\dot{\gamma}(t), \Hess g L^1(\gamma(t)) \dot{\gamma}(t)) + g \left( \frac{D}{dt} \dot{\gamma}(t), \nabla g L^1(\gamma(t)) \right),$$

and since $\nabla g L^1(\gamma(0)) = \nabla g L^1(W) = 0$, it follows that $g(\dot{\gamma}(0), \Hess g L^1(W) \dot{\gamma}(0)) < 0$ if $\left. \frac{d^2}{dt^2} L^1(\gamma(t)) \right|_{t=0} < 0$ and hence that $\Hess g L^1(W)$ has a negative eigenvalue in this case. (Note that $\Hess g L^1(W)$ is self-adjoint with respect to the scalar product $g$ on $T_W(M_r)$ and that it cannot be positive semidefinite (wrt. $g$) if $g(\dot{\gamma}(0), \Hess g L^1(W) \dot{\gamma}(0)) < 0$, hence it has a negative eigenvalue in this case.)

We note that $L^1(\gamma(t)) = \frac{1}{2} \| (\gamma(t) - I_d) X \|^2_F = \frac{1}{2} \tr(\gamma(t)^T \gamma(t) XX^T - 2\gamma(t)^T XX^T + XX^T)$. Since by construction we have $\gamma(t)^T = \gamma(t)^T \gamma(t)$ for all $t \in (-1, 1)$, we obtain

$$\| (\gamma(t) - I_d) X \|^2_F = \tr(-\gamma(t) XX^T + XX^T).$$

Let $\lambda_i$ be the eigenvalue of $XX^T$ corresponding to $u_i$, and $\lambda_0$ be the eigenvalue corresponding to $u_0$. Then it follows that

$$\| (\gamma(t) - I_d) X \|^2_F = (-t^2 \lambda_0 - (1-t^2) \lambda_i) + \tr(- \sum_{j=1, j \neq i}^{r} u_j u_j^T XX^T + XX^T).$$

(Note here that $\tr(u_i u_i^T XX^T) = \tr(u_0 u_0^T XX^T) = 0$.) Hence

$$\left. \frac{d^2}{dt^2} L^1(\gamma(t)) \right|_{t=0} = \lambda_i - \lambda_0 < 0.$$

This concludes the proof. 

\[\Box\]

Theorem 31. Assume that $Y = X$ and that $XX^T \in \mathbb{R}^{d \times d}$ has full rank. Let $r \leq d$ and $N \geq 2$ be positive integers and consider the Riemannian manifold $M_r$ with the metric $g$ given by [29]. Then there is a subset $N \subseteq M_r$ of measure zero such that for all $W_0 \in M_r \setminus N$ the flow

$$\dot{W} = -\nabla g L^1(W), \quad W(0) = W_0$$

converges to a global minimizer of $L^1$ on $M_r$.

In particular, given integers $d_1, \ldots, d_{N-1} \geq r$ and given balanced initial values $W_j(0) \in \mathbb{R}^{d_j \times d_j-1}$ for $j = 1, \ldots, N$ (where $d_N = d_0 = d$) such that $W(0) := W_N(0) \cdots W_1(0) \in M_r \setminus N$, under the flow [2], the matrix $W(t) := W_N(t) \cdots W_1(t)$ converges to a global minimizer of $L^1$ on $M_r$.

Proof. Given $W_0$, choose $d_1, \ldots, d_{N-1} \geq r$, let $d_0 = d_N = d$ and choose balanced initial values $W_j(0) \in \mathbb{R}^{d_j \times d_j-1}$ for $j = 1, \ldots, N$ such that $W_0 = W_N(0) \cdots W_1(0)$ (e.g., using the procedure described in [3] Section 3.3). By Theorem 12 under the flow [2], all $W_j$ converge to zero and all $W_j$ converge to some limit matrix, hence also $W$ converges to zero and $W(t)$ converges to a critical point of $L^1$ on $M_r$. By Proposition 30 all
critical points are strict saddle points except for the global minimizers. By Theorem 20 strict saddles are avoided for almost all initial points, which altogether means that the flow converges to a global minimizer for almost all initial points.

We conjecture a more precise version of the previous result in the spirit of Theorem 17.

**Conjecture 32.** Consider the autoencoder case where $X = Y$ and $N > 2$ with balanced starting conditions. Let $r = \min_{i=1,\ldots,N} d_i$. Let $\lambda_1 \geq \ldots \geq \lambda_d$ be the eigenvalues of $XX^T$ and let $u_1,\ldots,u_d$ be corresponding orthonormal eigenvectors. Let $U_r$ be the matrix with columns $u_1,\ldots,u_r$. Assume that $XX^T$ has full rank and that $\lambda_r > \lambda_{r+1}$. Assume further that $W(0)U_r$ has rank $r$ and that for all $i \in \{1,\ldots,r\}$ we have

$$u_i^T W(0) u_i > 0,$$

where $W(t) = W_N(t) \cdots W_1(t)$. Then $W(t)$ converges to $\sum_{i=1}^r u_i u_i^T$.

**Remark 33.** Without the condition that $u_i^T W(0) u_i > 0$ for all $i \in \{1,\ldots,r\}$, the above conjecture is wrong.

**Proof.** Indeed, in the case $N = 2$ and $r = 1$ with $W_1(0) = u_1^T$ and $W_2(0) = -u_1$ (which is a balanced starting condition and $W(0)U_1$ has obviously rank 1), we show that $W_1, W_2$ and $W$ all converge to the zero-matrix of their respective size. Write $W_1 = (\alpha_1,\ldots,\alpha_d)$ and $W_2 = (\beta_1,\ldots,\beta_d)^T$. We may assume that $XX^T$ is a diagonal matrix with entries $\lambda_1 \geq \ldots \geq \lambda_d > 0$. (In particular, the $u_i$ are given by the standard unit vectors $u_i = e_i$.) Then the system (43) becomes

$$\dot{\alpha}_j = -\lambda_j \alpha_j \sum_{i=1}^d \beta_i^2 + \lambda_j \beta_j, \quad \alpha_j(0) = \delta_{j1},$$

$$\dot{\beta}_j = -\beta_j \sum_{i=1}^d \lambda_i \alpha_i^2 + \lambda_j \alpha_j, \quad \beta_j(0) = -\delta_{j1}.$$

This system is solved by the following functions:

$$\alpha_1(t) = \frac{1}{\sqrt{2e^{2\lambda_1 t} - 1}}, \quad \alpha_j(t) = 0 \quad \text{for all } j \geq 2,$$

$$\beta_1(t) = \frac{-1}{\sqrt{2e^{2\lambda_1 t} - 1}}, \quad \beta_j(t) = 0 \quad \text{for all } j \geq 2.$$

Obviously, all $\alpha_j$ and $\beta_j$ converge to 0 as $t$ tends to infinity. From this the claim follows. (By Theorem 23 this equilibrium is not stable, so this behavior may not be obvious in numerical simulations.)

We further conjecture that convergence of the flow to global minimizers holds also for almost all starting points that are not necessary balanced. Moreover, we conjecture that these claims hold true for the non-autoencoder case $Y \neq X$.

7. Numerical results

In these experiments we numerically study the convergence of gradient flows in the linear autoencoder setting as a proof of concept of the convergence results presented above in the special case of autoencoders. Furthermore, the experiments also computationally explore the conjecture of the manuscript, Conjecture 32.

The experiment setup is as follows. The data matrix $X \in \mathbb{R}^{d_x \times m}$ is generated with columns drawn i.i.d. from a Gaussian distribution, i.e., $x_i \sim N(0,\sigma^2 I_d)$. Random realization of $X$ with sizes $d_x = d$ and $m = 3d$ varied to investigate different dimensions of the input data, i.e., with $10 \leq d \leq 50$. We study the gradient flow (5) in the autoencoder setting where $Y = X$ in (11) for three different values of $N$ (that is number of hidden layers in the autoencoder), precisely $N = 2,3,4$. A simple Euler method is used to solve the gradient flow differential equation with appropriate step sizes $t_n = t_0 + nh$ for large $n$ and $h \in (0,1)$. The experimental results can be categorized into three categories based on initial conditions of the gradient flow: a) general balanced – where the balanced conditions are satisfied and condition (17) of Conjecture 32 is satisfied; b) non-balanced – where the balanced conditions are not satisfied and c) special balanced – where the balanced conditions are satisfied but condition (17) of Conjecture 32 is not satisfied. In summary,
considering $W = W_N \cdots W_1$ as the limiting solution of the gradient flow, that is $W = \lim_{t \to \infty} W(t)$, where $W(t) = W_N(t) \cdots W_1(t)$. We show that the solutions of the gradient flow converges to $U_r U_r^T$, where the columns of $U_r$ are the $r$ eigenvectors corresponding to the $r$ largest eigenvalues of $X X^T$.

**a) General balanced initial conditions.** In this part we consider a general case of the balanced initial conditions, i.e., $W_{j+1}(0)W_j(0) = W_j(0)W_{j+1}(0), \ j = 1, \ldots, N - 1$, where condition 1.17 of Conjecture 5.2 is satisfied. The dimensions of the $W_j$ and their initializations are as follows.

- **Case $N = 2$:** Here, $W_1 \in \mathbb{R}^{d_1 \times d}$ and $W_2 \in \mathbb{R}^{d_2 \times d_1}$, where $d_1 = r$ is the rank of $W = W_2 W_1$ and $d_2 = d$. We initialize $W_1(0) = V_r^T$ where $V_r^T V_r = I_d$, and $W_2(0) = \tilde{V} W_1(0)^T = \tilde{V} V_r$ where $\tilde{V}^T \tilde{V} = I_d$.

- **Case $N > 2$:** Here, $W_i \in \mathbb{R}^{d_i \times d_{i-1}}$ for $i = 1, \ldots, N$ where $d_N = d_0 = d_e = d$ and $d_i = r$ is the rank of $W = W_N \cdots W_1$. We randomly generate $W(0) \in \mathbb{R}^{d \times d}$ with i.i.d. $w_{ij} \sim N(0, \sigma^2)$, where $\sigma = 1/\sqrt{d}$. Then compute the SVD of $W(0)$ as $U_0 \Sigma V_0^T$. We form $W_i(0) = V_i \Sigma_i^{1/N} V_{i-1}^T$ for $i = 1, \ldots, N - 1$, and $W_N(0) = U_0 \Sigma_i^{1/N} V_{N-1}^T$, where $U_0, V_0$ and $\Sigma$ are from the SVD of $W(0)$ and $\Sigma_i^{1/N}$ the $i$th root of the sub-matrix composed of the first $d_i$ rows and first $d_i$ columns of $\Sigma$. All the $V_i \in \mathbb{R}^{d_i \times d_i}$, for $i = 1, \ldots, N - 1$, are randomly generated orthogonal matrices.

**Figure 1.** Convergence of solutions for the general balanced case. Error between $W(t)$ and $U_r U_r^T$ (the top $r$ eigenvectors of $X X^T$) for different $r$ and $d$ values. **Left panel:** $N = 2$; **middle panel:** $N = 3$; and **right panel:** $N = 4$.

For all the values of $N$ and the different ranks of $W$ considered, Figure 1 shows that the limiting value of $W(t)$ as $t \to \infty$ is $U_r U_r^T$, where the columns of $U_r$ are $r$ eigenvectors of $X X^T$ corresponding to the largest $r$ eigenvalues of $X X^T$. This agrees with the theoretical results obtained for the autoencoder setting.

**Figure 2.** Convergence of solutions. **Left panel:** For $N = 2$, error between $W_2(t)$ and $W_2^T(t)$; **middle and right panels:** errors of the numerical solutions for $N = 3$ and $N = 4$ respectively.

Moreover, in the autoencoder setting when $N = 2$ we showed that $W_2 = W_1^T$. This is also tested and confirmed in the numerics as can be seen in the left panel plot of Figure 2. In addition, when $W(t)$ converges to $U_r U_r^T$ then $\|X - W(t)X\|_F$ converges to $\sqrt{\sum_{i=r+1}^N \sigma_i^2}$. This is also tested and confirmed for $N = 3, 4$ as
can be seen from the middle and right panel plots of Figure 2. This shows convergence of the functional $L^1(W(t))$ to the optimal error, which is the square-root of the sum of the tail eigenvalues of $XX^T$ of order greater than $r$.

b) Non-balanced initial conditions. In this part we only consider the case $N = 2$ as the case $N > 2$ is very similar to the former case. Note that we do not have theoretical results about convergence to global minimizers of solutions with non-balanced initial conditions. However, we attempt to investigate this numerically and we see similar results to the balanced case. For $W_1(0)$ and $W_2(0)$ we randomly generate Gaussian matrices. The plot in the left panel of Figure 3 shows that $W_2(t)$ converges to $W^T_1(t)$ even with non-balanced initial conditions. Moreover, similar to the settings with balanced initial conditions the solutions of the flow with non-balanced initial conditions still converge to $U_rU^T_r$, the outer product of the matrices containing the top $r$ eigenvectors of $XX^T$.

c) Special balanced initial conditions. Here we attempt to test Conjecture 32 by constructing pathological examples where we have balanced initial conditions, but $W(0)$ violates condition (47) of Conjecture 32. Precisely, we take $W_1(0) = V^T_r$ and $W_2(0) = -V_r$ where $V_r$ is the top $r$ eigenvectors of $XX^T$. This $W(0)$ clearly violates the condition of the conjecture $u^T_iW(0)u_i > 0$ for all $i \in [r]$. The hypothesis is that in such a setting the solution will not converge to the optimal solution proposed in Conjecture 32. Remark 33 showed that in such a case the solution should converge to 0, i.e., $\lim_{t \to \infty} W(t) = 0$. This can be seen in the left panel plot of Figure 4. The dip in the left panel shows that $W(t)$ was approaching zero. However, due to numerical errors the flow escapes the equilibrium point at zero. The right panel plot of Figure 4 shows convergence to $U_rU^T_r$. In fact, zero is an unstable point, so that, numerically, the flow will hardly converge to zero.
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