Robust and Resource Efficient Identification of Shallow Neural Networks by Fewest Samples

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Abstract

We address the structure identification and the uniform approximation of sums of
ridge functions $f(x) = \sum_{i=1}^{m} g_i(a_i \cdot x)$ on $\mathbb{R}^d$, representing a general form of a shallow
feed-forward neural network, from a small number of query samples. Higher order
differentiation, as used in our constructive approximations, of sums of ridge functions or
of their compositions, as in deeper neural network, yields a natural connection between
neural network weight identification and tensor product decomposition identification.
In the case of the shallowest feed-forward neural network, second order differentiation
and tensors of order two (i.e., matrices) suffice as we prove in this paper. We use two
sampling schemes to perform approximate differentiation - active sampling, where the
sampling points are universal, actively, and randomly designed, and passive sampling,
where sampling points were preselected at random from a distribution with known
density. Based on multiple gathered approximated first and second order differentials,
our general approximation strategy is developed as a sequence of algorithms to perform
individual sub-tasks. We first perform an active subspace search by approximating the
span of the weight vectors $a_1, \ldots, a_m$. Then we use a straightforward substitution, which
reduces the dimensionality of the problem from $d$ to $m$. The core of the construction
is then the stable and efficient approximation of weights expressed in terms of rank-1
matrices $a_i \otimes a_i$, realized by formulating their individual identification as a suitable
nonlinear program. We prove the successful identification by this program of weight
vectors being close to orthonormal and we also show how we can costructively reduce
to this case by a whitening procedure, without loss of any generality. We finally discuss
the implementation and the performance of the proposed algorithmic pipeline with
extensive numerical experiments, which illustrate and confirm the theoretical results.

Keywords: training shallow neural networks, breaking the curse of dimensionality,
randomized algorithms, whitening, nonlinear programming for optimizations in matrix sub-
spaces

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1 Introduction and main results

1.1 Introduction

In the last decade, deep neural networks (NN) outperformed other pattern recognition methods, achieving even superhuman skills in some domains [13, 37, 56]. In the meanwhile, the success of NNs has been further confirmed in speech recognition [24], optical character recognition [8], games solution [46, 54] and many other areas. Unfortunately, training a neural network usually involves a non-convex optimization and the process may get stuck.

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at one of the many of its local minimizers. Furthermore, due to the huge number of parameters of multi-layer NNs and the multitude of local minimizers, the performance of a neural network is often difficult to explain and interpret. This black-box feature makes often NNs not the first-choice machine learning method in those areas, where interpretability is a crucial issue (like security, cf. [11]) or for those applications where one wants to extract new insights from data [61].

It is therefore of interest to know, which neural networks can be uniquely determined in a stable way by finitely many training points. In fact, the unique identifiability is clearly a form of interpretability. The motivating problem of this paper is the robust and resource efficient training of feed forward neural networks [29, 30]. Unfortunately, it is known that training a very simple (but general enough) neural network is indeed NP-hard [5, 34]. Even without invoking fully connected neural networks, recent work [23, 42] showed that even the training of one single neuron (ridge function or single index model) can show any possible degree of intractability. Recent results [3, 35, 43, 55, 60], on the other hand, are more encouraging, and show that minimizing a square loss of a (deep) neural network does not have in general or asymptotically (for large number of neurons) poor local minima, although it may retain the presence of critical saddle points.

In this paper we present conditions for a shallow neural network to be provably and constructively identifiable with a number of samples, which is polynomially depending on the dimension of the network. Moreover, we prove that our procedure is robust to perturbations. Our results hold with uniform approximation. For the implementation we do not require high dimensional optimization methods and no concerns about complex energy loss landscapes need to be addressed, but only classical and relatively simple calculus and linear algebra tools are used (mostly function differentiation and singular value decompositions).

1.2 Ridge functions and tensor decompositions

We focus in particular on shallow feed forward neural networks

\[ \sum_{i=1}^{m} \alpha_i \sigma \left( \sum_{j=1}^{m} w_{ij} x_j + \theta_i \right), \]  

which constitute the main building blocks of deeper nets. To approach this problem, we study the more general task of the identification from minimal point queries of sums of ridge functions of the type

\[ \sum_{i=1}^{m} g_i(a_i \cdot x), \quad x \in \mathbb{R}^d, \]  

for some functions \( g_i : \mathbb{R} \to \mathbb{R} \) and some non-zero vectors \( a_i \in \mathbb{R}^d \). We assume that the functions \( g_i \) and the weights (or ridge directions) \( a_i \)'s are both unknown. Ridge function approximation has been extensively studied in mathematical statistics under the name of projection pursuit, see for instance [20, 31, 38]. The identification of sums of ridge functions has also been thoroughly considered in the approximation theory [10, 14, 15, 16, 18, 23, 39, 40, 41, 42, 50, 51], in particular we mention the work [9], where higher order differentiation was used to “extract” from the function \( f \) and “test” its principal directions \( a_i \)'s against
some given vectors $c_j$’s:

$$D^\alpha_1 \ldots D^\alpha_k c_j f(x) = \sum_{i=1}^{m} g_i^{(\alpha_1 + \ldots + \alpha_k)} (a_i \cdot x)(a_i \cdot c_i)^{\alpha_1} \ldots (a_i \cdot c_k)^{\alpha_k},$$

where $k \in \mathbb{N}$, $c_i \in \mathbb{R}^d$, $\alpha_i \in \mathbb{N}$ for all $i = 1, \ldots, k$ and $D^\alpha_i c_j$ is the $\alpha_i$-th derivative in the direction $c_i$. Hence, differentiation establishes a direct link between identification of the weights $a_i$’s and tensor decompositions [25]. Interestingly, [45] shows that learning the weights of a simple neural network (which essentially coincides with (1.2)) is as hard as the problem of decomposition of a tensor built up from these weights.

In order to avoid instability due to numerical differentiation and active sampling (active choice of point queries), “weak differentiation” approaches have been proposed. Let us describe the main ideas: Given an empirical sampling of points $x_k \sim \mu$ according to a probability distribution $\mu$, several methods, such as Stein’s lemma and differentiation by parts with respect to known density $p(x)$ of $\mu$ [33, 38], have been considered to build from point queries empirical approximations to tensors corresponding to the expected value of higher order derivatives, for instance

$$\Delta_2^k(f) = \frac{1}{N} \sum_{i=1}^{N} f(x_i)(-1)^k \frac{\nabla^k p(x_i)}{p(x_i)} = \int_{\mathbb{R}^d} f(x)(-1)^k \frac{\nabla^k p(x)}{p(x)} p(x) dx = \int_{\mathbb{R}^d} \nabla^k f(x) d\mu(x) = \mathbb{E}_{x \sim \mu}[\nabla^k f] = \sum_{i=1}^{m} \left( \int_{\mathbb{R}^d} g^{(k)}(a_i \cdot x) d\mu(x) \right) a_i \otimes \cdots \otimes a_i.$$

In the case of second order tensors, i.e., $k = 2$ this approach comes under the name of principal Hessian directions [38]. This case is particularly relevant, because it deals with empirical approximation of matrices of the type

$$\Delta_2^2(f) \approx \sum_{i=1}^{m} \int_{\mathbb{R}^d} g''(a_i \cdot x) d\mu(x) a_i \otimes a_i.$$

In case of orthogonal weights $a_i$’s and $m \leq d$, the identification of the weights is in principal solvable by spectral decomposition. However, this method leaves open the issue of dealing with non-orthogonal weights and the overdetermined case of $m > d$. In order to tackle both these issues the idea has been extended to third order tensors ($k = 3$) and tensor decompositions. Using precisely the approximation (1.3), in the recent paper [33] the authors proposed and analyzed the algorithm NN-LIFT, which learns a two-layer feed-forward neural network, where the second layer has a linear activation function. These results build upon the work [2] where symmetric non-orthogonal tensor decompositions are shown to be tractably computable. The non-orthogonal case is in fact addressed by reducing it via an orthogonalization procedure, called whitening, to the symmetric orthogonal tensor decomposition, which is known to be tractable [36, 59].

The approaches based on the approximation (1.3), e.g., both the principal Hessian directions [38] and the recent one in [33] for third order tensors, may suffer from a significant drawback: they are based on the decomposition of one single instance matrix/tensor, which is the empirical approximation to the expected value of (higher order) weak derivatives. In
fact, it is well known that spectral and tensor decompositions are in general unstable processes, unless spectral gaps and well-conditioning are guaranteed [58]. The error estimates appearing in [38, 33] look very similar, see, e.g., [38, Theorem 4.1] and [33, Theorem 3, formula (12) or Lemma 9, Lemma 10], and contain inverse proportional terms with respect to eigenvalues or tensor coefficients (with higher order power in the case of tensors), on which no control can be provided, unless one assumes well-conditioning a priori. In other words, if the one matrix/tensor at hand happens to have unstable decomposition, then one is simply left with bad luck. One may argue that this situation may generically not occur, but no proof is provided so far.

Another drawback of [38], as mentioned above, is that the approach via principal Hessian directions cannot deal with non-orthogonal weights. In the paper [33] the authors claim that, while a matrix decomposition is only identifiable up to orthogonal components, tensors can have identifiable non-orthogonal components and use this argument to motivate the necessity of the complexity and potential higher instability of third order tensors. Unfortunately, the low-rank tensor decomposition problem is usually not well-posed [17]. (This is based on the result that there are rank-$(r + 1)$ tensors in the closure of rank-$r$ tensors.) Nonetheless, in certain regimes and under certain assumptions, also for $m$-rank tensors with $m > d$ and without assumptions of near-orthonormality, it is uniquely solvable. A very helpful characterization of the regime where tensor decomposition is a well-posed problem can be given in terms of the generic rank $r_{\text{gen}}(d, s)$: if $m \leq r_{\text{gen}}(d, s) := \frac{1}{d + 1} \left( \frac{d + s}{s} \right)$ then with the exception of nongeneric cases, every $m$-rank $s$-tensor in $\mathbb{R}^d$ has a unique rank-$m$ decomposition (up to rescaling); moreover there are algorithms to find such a decomposition, mainly based on algebraic methods [12, 44, 48], whose stability under perturbation is presently not known.

In this paper we approach the problem of the weight identification by using a robust procedure, which does not suffer from the potential instabilities of being based on a single matrix/tensor instance as in [33, 38]. Moreover, we disprove the claim that it is necessary to use higher order tensors in order to deal with non-orthogonal weights: in fact, by developing an appropriate whitening procedure, we will exclusively build our identification procedure on matrices, making our approach resource efficient and potentially more stable than tensor technology, which is in general more susceptible to intractability and instabilities [17, 27, 28]. Also in our error estimates, see, e.g., (2.15), (3.9), we require inverse proportional terms with respect to conditioning of the problem encoded by constants $\alpha, \alpha_2$; however, as we use a lower order differentiation and matrices (not tensors), the power magnitude of these terms is smaller than for higher order differentiations and tensors as in, e.g., [33, Theorem 3, formula (12) or Lemma 9, Lemma 10], where such terms appear even at the sixth power. In this paper we focus on the case of $m \leq d$. In [22] we are addressing the overdetermined case of $m > d$ and of two hidden layer$^1$ feed-forward neural networks, inspired by layer-by-layer procedures [4, 29].

1.3 Dimensionality reduction

The approach we are intending to follow is dictated by the following result, whose proof we report in more detail in Section 2.

$^1$In view of a certain ambiguity in the literature, we clarify that, for two hidden layers, we mean here one more fully nonlinear layer with respect to (1.1).
Theorem 1.1 (Reduction to $m$ dimensions). Let us consider a function
\[
f(x) = \sum_{i=1}^{m} g_i(a_i \cdot x), \quad x \in B_1^d = \{x \in \mathbb{R}^d : \|x\|_2 \leq 1\},
\]
for $m \leq d$ and we denote $A = \text{span}\{a_1, \ldots, a_m\}$.

Let us now fix a $m$-dimensional subspace $\tilde{A} \subset \mathbb{R}^d$, whose we choose an orthonormal basis $\{b_1, \ldots, b_m\}$, so that $A = \text{span}\{b_1, \ldots, b_m\}$. We arrange the vectors $b_i$'s as columns of a matrix $B$, and we denote with $P_A$ and $P_{\tilde{A}}$ the orthogonal projections onto $A$ and $\tilde{A}$ respectively. Then one can construct a function
\[
\tilde{f}(y) = \sum_{i=1}^{m} \tilde{g}_i(\alpha_i \cdot y), \quad y \in B_1^m \subset \mathbb{R}^m,
\]
with $\alpha_i = B^T a_i$, such that for any other function $\hat{f} : \mathbb{R}^m \to \mathbb{R}$ the following estimate holds
\[
\|f - \tilde{f}(B^T \cdot)\|_{\infty} \leq \|f\|_{\text{Lip}} \|P_A - P_{\tilde{A}}\|_F + \|\tilde{f} - \hat{f}\|_{\infty}. \tag{1.6}
\]
Moreover, for any other set of vectors $\{\tilde{\alpha}_1, \ldots, \tilde{\alpha}_m\} \subset \mathbb{R}^m$,
\[
\|a_i - B\tilde{\alpha}_i\|_2 \leq \|P_A - P_{\tilde{A}}\|_F + \|\alpha_i - \tilde{\alpha}_i\|_2. \tag{1.7}
\]

In view of (1.5), (1.6), and (1.7), the approximation of a sum of $m$ ridge functions (1.4) on $\mathbb{R}^d$ and the identification of its ridge directions can be reduced to the approximation of a sum of $m$ ridge functions (1.5) on $\mathbb{R}^m$ and the identification of its ridge directions, as soon as one can approximate well the subspace $A$ by means of any other subspace $\tilde{A}$. Hence, we need to focus on two relevant tasks. The first one is the approximation of the subspace $A$ and the second is the identification of ridge directions of a sum of ridge functions defined on $B_1^m \subset \mathbb{R}^m$. We approach the problem of approximating the subspace $A$ both by active sampling in order to seek for minimal number of point queries, and passive sampling, by suitable generalizations of (1.3), to deal with more realistic scenarios, where only noisy arbitrary samples are given. The main idea for both active and passive sampling is computing $m_\mathcal{X} \in \mathbb{N}$ approximations to “classical or weak gradients” of $f$ of the type
\[
Y_j \approx \sum_{i=1}^{m} S_j(g'(a_i \cdot \cdot)) a_i, \quad j = 1, \ldots, m_\mathcal{X},
\]
where $S_j$ are suitable linear operators (including sampling operators). Under suitable conditions, which we will make clear below, $\tilde{A} = \text{span}\{Y_1, \ldots, Y_{m_\mathcal{X}}\}$ will form an approximating subspace to $A$. As an example of results, in case $S_j$ is an (active) sampling operator, i.e., $S_j(g'(a_i \cdot \cdot)) = g'(a_i \cdot x_j)$ for $x_j$ generated at random on the sphere $\mathbb{S}^{d-1}$, Algorithm 2.1 requires that the matrix
\[
J[f] := \int_{\mathbb{S}^{d-1}} \nabla f(x) \nabla f(x)^T d\mu_{\mathbb{S}^{d-1}}(x)
\]
has full rank $m$, being $\mu_{\mathbb{S}^{d-1}}$ the uniform measure on the sphere $\mathbb{S}^{d-1}$. It computes an approximating subspace $\tilde{A}$ by using $m_\mathcal{X}(d+1)$ point evaluations of $f$ with high probability, increasing exponentially to one with the number $m_\mathcal{X}$ of samples on the sphere.

\[\text{With a certain abuse of notation, we often use in this paper the symbol } A \text{ also to denote the matrix whose columns are the vectors } \{a_1, \ldots, a_m\}.\]

\[\text{The use of the uniform measure on the sphere for active sampling is by no means a restriction, more general distributions could be used with no significant difference in the results.}\]
1.4 Weight identification

As soon as an approximating space $\tilde{A}$ of $A$ has been identified, we can then apply Theorem 1.1 and reduce the dimensionality of the problem to $d = m$. It remains to find a way of approximating the ridge directions of a sum of ridge functions in $R^m$. We approach this latter issue in Section 3.1 (cf. Algorithm 3.1) by first finding an approximating matrix space $\tilde{A} \in R^{m \times m}$ to $A = \text{span}\{a_1 \otimes a_1, \ldots, a_m \otimes a_m\}$. This is the main fundamental difference with respect to [2, 38] as we are not simply content with one (vector or matrix) instance, which might have unstable decomposition, but we are building an entire subspace where to search for the good one. Again the idea is to construct via active or passive sampling approximations

$$Y_j \approx \sum_{i=1}^{m} S_j(g''(a_i \cdot )) a_i \otimes a_i, \quad j = 1, \ldots, m \chi,$$

where $S_j$ are suitable linear operators (including sampling operators). As an example of results, in the case of active sampling, the result (Theorem 3.2) resembles very much the one for the identification of $A = \text{span}\{a_1, \ldots, a_m\}$ provided by Algorithm 2.1 and it reads as follows: if the matrix $H_2[f] := \int_{S^{m-1}} \text{vec}(\nabla^2 f(x)) \otimes \text{vec}(\nabla^2 f(x)) d\mu_{S^{m-1}}(x)$ has full rank $m$ (the symbol $\text{vec}(\nabla^2 f(x))$ stands for the vectorization of the Hessian of $f$, see (3.3) for its precise definition), then Algorithm 3.1 based on second differentiation of $f$ provides an approximating matrix space $\tilde{A} \in R^{m \times m}$ to $A$ with arbitrary accuracy by using $m \chi(m + 1)(m + 2)/2$ point evaluations of $f$ with high probability, increasing exponentially to one with the number $m \chi$ of samples on the sphere.

If this approximation is fine enough, then we can assume $\tilde{A}$ to be spanned by near rank-1 matrices of unit Frobenius norm as well, and those to be good approximations to $a_1 \otimes a_1, \ldots, a_m \otimes a_m$. For identifying such a basis for $\tilde{A}$ we need to find in it elements of minimal rank. Let us stress that this problem is strongly related to similar and very relevant ones appearing recently in the literature addressing nonconvex programs to identify sparse vectors and low-rank matrices in linear subspaces, see, e.g., in [47, 52]. In fact, differently from [33, 38] we do not address an orthogonal decomposition of a single matrix of $\tilde{A}$, which might be subjected to instabilities, but we are searching within $\tilde{A}$ appropriate matrices, whose decomposition we prove to be robust and safe. We perform such a search by solving a nonlinear program, maximizing the spectral norm among competitors in $\tilde{A}$ of the Frobenius norm bounded by one, i.e.,

$$\text{arg max} \|M\|_\infty, \quad \text{s.t.} \quad M \in \tilde{A}, \|M\|_F \leq 1. \quad (1.8)$$

In Section 3.2 we characterize the solutions to the problem (1.8) by analyzing its first and second order optimality conditions. We analyze the optimization algorithm (1.8) under the assumptions that the ridge profiles $a_1, \ldots, a_m$ are $\varepsilon$-nearly-orthonormal, i.e. that they are close to some orthonormal basis of $R^m$ as described in the following definition.

**Definition 1.1.** Let $a_1, \ldots, a_m \in R^m$ be unit vectors. Then we define

$$S(a_1, \ldots, a_m) = \inf \left\{ \left( \sum_{i=1}^{m} \|a_i - w_i\|_2^2 \right)^{1/2} : w_1, \ldots, w_m \text{ orthonormal basis in } R^m \right\}. \quad (1.9)$$
We say that \( a_1, \ldots, a_m \in \mathbb{R}^m \) are \( \varepsilon \)-nearly-orthonormal, if \( S(a_1, \ldots, a_m) \leq \varepsilon \), for \( \varepsilon > 0 \) relatively small.

In Section 3.3 we prove that this assumption is without loss of generality, as we will be able to specify a whitening procedure (\( \varepsilon \)-near-orthonormalization) for matrices very much inspired by the ones described in [2, 33, 36] for symmetric tensors. Again, differently from [33], we will not rely on one instance matrix/tensor, but rather search within the space \( \tilde{A} \) for the right whitening matrix with the necessary stability properties.

We show in Section 3.4 that the local maximizers of (1.8) are actually close to \( \{a_1 \otimes a_1, \ldots, a_m \otimes a_m\} \) as soon as \( \tilde{A} \) is a good approximation to \( A \). In Section 3.5 we present an algorithm (Algorithm 3.4), which is easy to implement and which strives for the solution of this optimization problem, by a sort of iteratively projected gradient ascent, and we prove some of its convergence properties.

Once we have identified the approximations \( \{\hat{a}_1, \ldots, \hat{a}_m\} \) of \( \{a_1, \ldots, a_m\} \) by Algorithm 3.3 or Algorithm 3.4, the final step addressed in Section 3.4 is then to approximate the functions \( g_1, \ldots, g_m \) by \( \hat{g}_1, \ldots, \hat{g}_m \). The approximation of \( f \) is then given by Algorithm 4.1 as follows

\[
\hat{f}(x) = \sum_{i=1}^{m} \hat{g}_i(\hat{a}_i \cdot x), \quad x \in B^m_1.
\]

At this point, it is worth to summarize all the construction through the different algorithms in a single higher level result, which we specify for the case of active sampling. We use the notations introduced so far.

**Theorem 1.2.** Let \( f \) be a real-valued function defined on the neighborhood of \( B^d_1 \), which takes the form

\[
f(x) = \sum_{i=1}^{m} g_i(a_i \cdot x),
\]

for \( m \leq d \). Let \( g_i \) be three times continuously differentiable on a neighborhood of \([-1,1]\) for all \( i = 1, \ldots, m \), and let \( \{a_1, \ldots, a_m\} \) be linearly independent. We additionally assume both \( J[f] \) and \( H_2[f] \) of maximal rank \( m \). Then, for all \( \varepsilon > 0 \), using at most \( m \chi[(d + 1) + (m + 1)(m + 2)/2] \) random exact point evaluations of \( f \), Algorithms 2.1-3.2 construct approximations \( \{\hat{a}_1, \ldots, \hat{a}_m\} \) of the ridge directions \( \{a_1, \ldots, a_m\} \) up to a sign change for which

\[
\left( \sum_{i=1}^{m} \|\hat{a}_i - a_i\|^2 \right)^{1/2} \lesssim \varepsilon, \tag{1.10}
\]

with probability at least \( 1 - m \exp\left(-\frac{m \varepsilon^c}{\max(C_1, C_2)^2 m^2}\right) \), for a suitable constant \( c > 0 \) intervening (together with some fixed power of \( m \)) in the asymptotical constant of the approximation (1.10). Moreover, Algorithm 4.1 constructs an approximating function \( \hat{f} : B^d_1 \to \mathbb{R} \) of the form

\[
\hat{f}(x) = \sum_{i=1}^{m} \hat{g}_i(\hat{a}_i \cdot x),
\]

such that

\[
\|f - \hat{f}\|_{L_\infty(B^d_1)} \lesssim \varepsilon. \tag{1.11}
\]
In absence of noise on the point evaluations of \( f \) as in Theorem 1.2, the usage of more point evaluations does not improve the accuracy in (1.10) and (1.11), but only the probability of success, and the result holds true with arbitrary accuracy, exclusively depending on the way active sampling is used to approximate derivatives by finite differences. The result would need to be significantly modified in case of noise on the active point evaluations of \( f \) in order to deal with stability issues determined by employing finite differences in order to approximate the gradient and the Hessian of \( f \). Contrary to most results available in the literature \([3, 33, 43, 60]\), our final estimate (1.11) holds in the uniform norm, which is deterministic once the weights are correctly identified. In fact, probabilistic least squares error estimates usually investigated in the literature may appear to successfully circumvent the curse of dimensionality, but they are obtained at the practically relevant price of not ensuring uniform error bounds. Not only we avoid the curse of dimensionality, but we also do not compromise on the uniform bound.

In the setting of passive sampling, we assume that the values \( f(x_1), \ldots, f(x_{m_X}) \) were sampled in points \( x_1, \ldots, x_{m_X} \), which are chosen independently with respect to a probability distribution \( \mu \) on \( B^d_1 \). Here, we assume that its density \( p(x) \) is smooth and known in advance. Using Stein’s lemma \([57]\) or integration by parts in a way similar to \([33]\) and \([38]\), we transfer our analysis also to the setting of passive sampling, leading first to the reduction of dimension from \( d \) to \( m \leq d \) and then to the approximation of \( A = \text{span}\{a_1 \otimes a_1, \ldots, a_m \otimes a_m\} \). Due to the non-local nature of the sampling process, it is rather easy to incorporate noise. Similarly to the active sampling, our main tools are the matrix concentration inequalities \([1, 49, 53, 63]\).

We conclude this introduction by mentioning that this paper, besides the specific application on identification of shallow neural networks, contains results of independent mathematical and computational interest. First of all, we proved that stable whitening of matrices is constructively attainable, see Section 3.3. This seems to disprove a common belief in the literature, see, e.g., \([33]\), that the use of third or higher order tensors can not be avoided. Moreover, we introduced a new nonconvex optimization (3.1) with no spurious local minimizers, which allows identifying robustly 1-rank matrices in linear subspaces of symmetric matrices, see Section 3.2 and Section 3.4. We provide a simple and efficient iterative algorithm to perform such an optimization, Section 3.5. Similar problems appeared recently in the literature and are of independent interest \([47, 52]\).

The notation used throughout the paper is rather standard. For \( 0 < p < \infty \), we denote by \( \|x\|_p = \left( \sum_{j=1}^d |x_j|^p \right)^{1/p} \) the \( p \)-(quasi)-norm of a vector \( x \in \mathbb{R}^d \). This notation is complemented by setting \( \|x\|_\infty = \max_{j=1,\ldots,d} |x_j| \). If \( M \in \mathbb{R}^{m \times d} \) is an \( m \times d \) matrix, Schatten-\( p \) norm \( \|M\|_p \) is defined as the \( p \)-norm of the vector of the singular values of \( M \). In particular we denote by \( \|M\|_F = \|M\|_2 \) the Frobenius norm, by \( \|M\| = \|M\|_\infty \) the spectral norm, and by \( \|M\|_* = \|M\|_1 \) the nuclear norm. The inner product of two vectors \( x, y \in \mathbb{R}^d \) is denoted by \( \langle x, y \rangle = x \cdot y = x^T y \). Their tensor product is a rank-1 matrix denoted by \( xy^T = x \otimes y \). More specific notation is introduced along the way, when needed.
2 Active subspace identification and dimensionality reduction

The aim of this paper is the structure identification and uniform approximation of sums of ridge functions

\[ f(x) = \sum_{i=1}^{m} g_i(a_i \cdot x), \quad x \in B_1^d. \]  

(2.1)

We assume throughout that the vectors \( a_1, \ldots, a_m \in \mathbb{R}^d \) are linearly independent and, therefore, \( m \leq d \). Nevertheless, the typical setting we have in mind is that the number \( d \gg 1 \) of variables is very large and the number \( m \) of summands in (2.1) might be smaller than \( d \), i.e. \( m \ll d \).

The main aim of this section is the proof of Theorem 1.1, which allows to reduce the general case \( m \leq d \) to \( d = m \), hence, with a potentially significant dimensionality reduction. Due to the typical range of parameters we have in mind, this step is crucial in reducing the complexity of the approximation of (2.1).

2.1 Reduction to dimension \( d = m \)

Proof of Theorem 1.1. Let us assume that the unknown function \( f : B_1^d \rightarrow \mathbb{R} \) takes the form of a sum of ridge functions (2.1) with unknown univariate functions \( g_i : [-1, 1] \rightarrow \mathbb{R} \) and unknown ridge profiles \( a_1, \ldots, a_m \in \mathbb{R}^d \). We denote \( A = \text{span}\{a_1, \ldots, a_m\} \).

We assume (and we shall discuss this point later in this section) that we were able to find a subspace \( \tilde{A} \subset \mathbb{R}^d \), which approximates \( A \). We select an (arbitrary) orthonormal basis \( (b_i)_{i=1}^{m} \) of \( \tilde{A} \), and consider the \( d \times m \) matrix \( B \) with columns \( b_1, \ldots, b_m \). Finally, we set \( \alpha_i = B^T a_i \in \mathbb{R}^m \) with \( \|\alpha_i\|_2 = \|P_A a_i\|_2 \leq 1 \).

We observe that the function

\[ \tilde{f}(y) := f(By) = \sum_{i=1}^{m} g_i(a_i \cdot By) = \sum_{i=1}^{m} g_i(\alpha_i \cdot y), \quad y \in B_1^m, \]

is a sum of \( m \) ridge functions on \( B_1^m \subset \mathbb{R}^m \). Furthermore, sampling of \( \tilde{f} \) can be easily transferred to sampling of \( f \) by \( \tilde{f}(y) = f(By) \). Let us assume that \( \tilde{f} \) is a uniform approximation of \( \hat{f} \) on \( B_1^m \). Then the function \( \hat{f}(B^T x) \) is a uniform approximation of \( f \) on \( B_1^d \). Indeed, let \( x \in B_1^d \). We have

\[
|f(x) - \hat{f}(B^T x)| \leq |f(x) - \tilde{f}(B^T x)| + |\tilde{f}(B^T x) - \hat{f}(B^T x)|
\leq |f(x) - f(BB^T x)| + \|\hat{f} - \tilde{f}\|_{\infty} = |f(P_A x) - f(P_A x)| + \|\tilde{f} - \hat{f}\|_{\infty}
\leq \|f\|_{\text{Lip}} \cdot \|P_A x - P_A x\|_2 + \|\tilde{f} - \hat{f}\|_{\infty}.
\]

If we take the supremum over \( x \in B_1^d \), we get

\[
\|f - \hat{f}(B^T \cdot)\|_{\infty} \leq \|f\|_{\text{Lip}} \cdot \|P_A - P_A\|_{\infty} + \|\tilde{f} - \hat{f}\|_{\infty}.
\]

A crucial step in the construction of the uniform approximation \( \hat{f} \) of \( \tilde{f} \) on \( B_1^m \) will be the identification of the ridge profiles \( \alpha_1, \ldots, \alpha_m \). Naturally, we will not be able to recover them exactly and we will only obtain some good approximation \( \{\tilde{\alpha}_1, \ldots, \tilde{\alpha}_m\} \subset \mathbb{R}^m \). Then the
vectors $B\hat{a}_i$ approximate well the original ridge profiles $a_i$ as can be observed by using $B\alpha_i = BB^T a_i = PAa_i$ and

$$
\|a_i - B\hat{a}_i\|_2 \leq \|a_i - B\alpha_i\|_2 + \|B(\alpha_i - \hat{\alpha}_i)\|_2 = \|(PA - P\hat{A})a_i\|_2 + \|B(\alpha_i - \hat{\alpha}_i)\|_2 \\
\leq \|PA - P\hat{A}\|_\infty + \|\alpha_i - \hat{\alpha}_i\|_2,
$$

which finishes the proof. □

Remark 1. Let $\{a_1, \ldots, a_m\}$ be $\varepsilon$-nearly orthonormal and let $\{w_1, \ldots, w_m\} \subset \mathbb{R}^d$ be an optimal approximating orthonormal basis such that

$$
S(a_1, \ldots, a_m) = \left(\sum_{j=1}^m \|a_j - w_j\|_2^2\right)^{1/2} = \varepsilon.
$$

By Theorem 6.2 (and its proof) we can assume that $\{w_1, \ldots, w_m\} \subset A$. Then

$$
S(\alpha_1, \ldots, \alpha_m) = S(B^T a_1, \ldots, B^T a_m) = S(BB^T a_1, \ldots, BB^T a_m) = S(P\hat{A}a_1, \ldots, P\hat{A}a_m) \\
\leq \left(\sum_{j=1}^m \|P\hat{A}a_j - w_j\|_2^2\right)^{1/2} + \left(\sum_{j=1}^m \|P\hat{A}w_j - PAw_j\|_2^2\right)^{1/2} \\
\leq \varepsilon + \|P\hat{A} - PA\|_F.
$$

Hence, if the vectors $a_1, \ldots, a_m$ are orthogonal, or nearly-orthonormal in the sense of Definition 1.1, the vectors $\alpha_1, \ldots, \alpha_m$ behave similarly.

### 2.2 Approximation of the span of ridge profiles

As previously shown, as soon as we can produce a subspace $\hat{A} \subset \mathbb{R}^d$ approximating $A = \text{span}\{a_1, \ldots, a_m\}$, we can eventually reduce the problem of approximating a sum of ridge functions in $\mathbb{R}^d$ to the same problem in $\mathbb{R}^m$, preserving even the quasi-orthogonality, cf. Remark 1. In this section we describe two different methods of identification of $A$. The first one applies to the setting of active sampling. It is motivated by the results in [23] and makes use of first order differences. The second method is inspired by [33], and implements passive sampling under the assumption that we dispose of the probability density $p(x)$ of the point distribution of the samples.

#### 2.2.1 Active sampling

We observe that the vector

$$
\nabla f(x) = \sum_{i=1}^m g_i'(a_i \cdot x)a_i
$$

lies in $A$ for every $x \in \mathbb{R}^d$. We consider (2.2) for different $x_1, \ldots, x_{m_X} \in \mathbb{R}^d$, where $m_X \geq m$. In a generic situation for the points $x_i$’s, $A$ is likely given as the span of $\{\nabla f(x_1), \ldots, \nabla f(x_{m_X})\}$.
As we would like to use only function values of $f$ in our algorithms, we use for every $j = 1, \ldots, d$ and every $k = 1, \ldots, m_X$ the Taylor’s expansion

$$
\frac{\partial}{\partial e_j} f(x_k) = \frac{f(x_k + \epsilon e_j) - f(x_k)}{\epsilon} - \left[ \frac{\partial}{\partial e_j} f(x_k + \eta_{j,k} e_j) - \frac{\partial}{\partial e_j} f(x_k) \right]
$$

(2.3)

for some $\eta_{j,k} \in [0, \epsilon]$. We recast the $d \times m_X$ instances of (2.3) into the matrix notation

$$
X = Y - E,
$$

(2.4)

where

$$
X_{j,k} = \frac{\partial}{\partial e_j} f(x_k), \quad Y_{j,k} = \frac{f(x_k + \epsilon e_j) - f(x_k)}{\epsilon},
$$

(2.5)

and

$$
E_{j,k} = \frac{\partial}{\partial e_j} f(x_k + \eta_{j,k} e_j) - \frac{\partial}{\partial e_j} f(x_k)
$$

for $j = 1, \ldots, d$ and $k = 1, \ldots, m_X$. It follows from (2.2), that $A$ is the linear span of columns of $X$. Naturally, we define $\tilde{A}$ using the linear span of the singular vectors of $Y$ corresponding to its $m$ largest singular values. This is formalized in the following algorithm.

**Algorithm 2.1.**

- Construct $Y$ according to (2.5).
- Compute the singular value decomposition of

$$
Y^T = \begin{pmatrix} \tilde{U}_1 & \tilde{U}_2 \end{pmatrix} \begin{pmatrix} \tilde{\Sigma}_1 & 0 \\ 0 & \tilde{\Sigma}_2 \end{pmatrix} \begin{pmatrix} \tilde{V}_1^T \\ \tilde{V}_2^T \end{pmatrix},
$$

where $\tilde{\Sigma}_1$ contains the $m$ largest singular values.
- Set $\tilde{A}$ to be the row space of $\tilde{V}_1^T$.

The aim of the rest of this section is to show, that $\tilde{A}$ constructed in Algorithm 2.1 is in some sense close to $A$. To be more specific, we need to bound $\|P_A - P_{\tilde{A}}\|$, i.e. the operator or the Frobenius norm of the difference between the orthogonal projections onto $A$ and $\tilde{A}$, respectively. For this first approximation method we need to introduce a new matrix

$$
J[f] := \int_{S^{d-1}} \nabla f(x) \nabla f(x)^T d\mu_{S^{d-1}}(x).
$$

**Lemma 2.1.** Assume the vectors $(a_i)_{i=1}^m$ linearly independent, and $\|a_i\|_2 = 1$ for all $i = 1, \ldots, m$. Additionally assume

$$
C_1 := \max_{i=1,\ldots,m} \max_{-1 \leq t \leq 1} |g_i'(t)| < \infty.
$$

Suppose that $\sigma_m(J[f]) \geq \alpha > 0$, i.e., the $m$th singular value of the matrix $J[f]$ is bounded away from zero. Then for any $s \in (0, 1)$ we have that

$$
\sigma_m(X) \geq \sqrt{m_X \alpha (1 - s)}
$$

(2.6)

with probability at least $1 - m \exp \left( - \frac{m_X \alpha^2 s^2}{2C_1^2 m^2} \right)$, where $X$ is constructed as in (2.4) for $x_1, \ldots, x_{m_X} \in S^{d-1}$ drawn uniformly at random.
Proof. The result will follow by a suitable application of Theorem 6.7 in the Appendix. Let $w_1, \ldots, w_m$ be an orthonormal basis of $A$. We denote $P^A = ((w_1 \cdot x), \ldots, (w_m \cdot x))^T \in \mathbb{R}^m$. We identify $P^A$ with the corresponding $m \times d$ matrix, i.e., the matrix with rows $w_1^T, \ldots, w_m^T$. We observe that $\sigma_j(X) = \sigma_j(P^A X) = \sqrt{\sigma_j(P^A X X^T (P^A)^T)}$,

$$XX^T = \sum_{l=1}^{mX} \nabla f(x_l) \nabla f(x_l)^T$$

and

$$P^A X X^T (P^A)^T = \sum_{l=1}^{mX} P^A \nabla f(x_l) \nabla f(x_l)^T (P^A)^T.$$  

Furthermore, we obtain for every $x \in \mathbb{R}^d$

$$\sigma_1(P^A \nabla f(x) \nabla f(x)^T (P^A)^T) = \sigma_1(\nabla f(x) \nabla f(x)^T) = \|\nabla f(x) \nabla f(x)^T\|_F$$

$$= \|\nabla f(x)^2 = \sum_{l=1}^{d} \left( \sum_{i=1}^{m} g_i'(a_i \cdot x) a_{i,l} \right)^2$$

$$\leq C_1^2 \sum_{l=1}^{d} \left( \sum_{i=1}^{m} |a_{i,l}| \right)^2 \leq C_1^2 \left( \sum_{i=1}^{m} \sum_{l=1}^{d} |a_{i,l}|^2 \right)^2 = C_1^2 m^2.$$  

Hence $X_j = P^A \nabla f(x_j) \nabla f(x_j)^T (P^A)^T$ is a random $m \times m$ positive-semidefinite matrix, that is almost surely bounded. Moreover,

$$\mathbb{E} X_j = P^A \int_{\mathbb{S}^{d-1}} \nabla f(x) \nabla f(x)^T d\mu_{\mathbb{S}^{d-1}}(x) (P^A)^T = P^A J[f] (P^A)^T.$$  

We conclude that $\mu_{\min} = \mu_{\min} \left( \sum_{j=1}^{mX} \mathbb{E} X_j \right) \geq mX \alpha$, and by Theorem 6.7 in the Appendix

$$\sigma_m(X) = \sqrt{\sigma_m(P^A X X^T (P^A)^T)} \geq \sqrt{\mu_{\min}(1-s)} \geq \sqrt{mX \alpha(1-s)}$$

with probability at least

$$1 - m \exp \left( - \frac{\mu_{\min} s^2}{2C_1^2 m^2} \right) \geq 1 - m \exp \left( - \frac{mX \alpha s^2}{2C_1^2 m^2} \right).$$

Remark 2. If we further assume that $a_1, \ldots, a_m$ are $\varepsilon$-nearly-orthonormal and $w_1, \ldots, w_m$ are orthonormal vectors with

$$S(a_1, \ldots, a_m) = \left( \sum_{i=1}^{m} \|a_i - w_i\|^2 \right)^{1/2} \leq \varepsilon,$$
we can improve (2.7) to
\[
\sigma_1(P^A \nabla f(x) \nabla f(x)^T (P^A)^T) \leq \|\nabla f(x)\|_2^2 = \left\| \sum_{i=1}^m g_i'(a_i \cdot x) a_i \right\|_2^2 \\
\leq \left( \left\| \sum_{i=1}^m g_i'(a_i \cdot x) w_i \right\|_2 + \left\| \sum_{i=1}^m g_i'(a_i \cdot x) (a_i - w_i) \right\|_2 \right)^2 \\
\leq \left[ \left( \sum_{i=1}^m |g_i'(a_i \cdot x)|^2 \right)^{1/2} + \sum_{i=1}^m |g_i'(a_i \cdot x)| \cdot \|a_i - w_i\|_2 \right]^2 \\
\leq (1 + \varepsilon)^2 \sum_{i=1}^m |g_i'(a_i \cdot x)|^2 \leq C_1^2 (1 + \varepsilon)^2 m.
\]

The rest of the proof then follows in the same manner, only the probability changes to
\[
1 - m \exp \left( -\frac{m \chi \alpha s^2}{2C_1^2 (1 + \varepsilon)^2 m} \right).
\]

The same remark applies also to Theorem 3.2 below.

The following theorem quantifies the distance between the subspace \( \tilde{A} \) constructed in Algorithm 2.1 and \( A \).

**Theorem 2.2.** Assume the vectors \( (a_i)_{i=1}^m \) are linearly independent, and \( \|a_i\|_2 = 1 \) for all \( i = 1, \ldots, m \). Additionally assume that
\[
C_1 := \max_{i=1,\ldots,m} \max_{-1 \leq t \leq 1} |g_i'(t)| < \infty
\]
and that the Lipschitz constants of all \( g_j' \), \( j = 1, \ldots, m \), are bounded by \( C_2 < \infty \).

Let \( \tilde{A} \) be constructed as described in Algorithm 2.1 by sampling \( m \chi (d + 1) \) values of \( f \). Let \( 0 < s < 1 \), and assume \( \sigma_m(J[f]) \geq \alpha > 0 \). Then
\[
\|P_A - P_{\tilde{A}}\|_F \leq \frac{2C_2 \varepsilon m}{\sqrt{\alpha (1 - s) - C_2 \varepsilon m}}
\]
with probability at least \( 1 - m \exp \left( -\frac{m \chi \alpha s^2}{2C_1^2 (1 + \varepsilon)^2 m} \right) \).

**Proof.** We intend to apply the so-called Wedin’s bound, as recalled in Theorem 6.6 in the Appendix, to estimate the distance between \( A \) and \( \tilde{A} \). If we choose \( B = X^T \) and \( \tilde{B} = Y^T \), we get \( \Sigma_2 = 0 \) and we observe that (6.2) and (6.3) are satisfied with \( \bar{\alpha} = \sigma_m(Y^T) \). Therefore, Theorem 6.6 implies
\[
\|P_A - P_{\tilde{A}}\|_F = \|V_1 V_1^T - \tilde{V}_1 \tilde{V}_1^T\|_F \leq \frac{2\|X - Y\|_F}{\sigma_m(Y^T)}
\]
\[
\leq \frac{2\|X - Y\|_F}{\sigma_m(X^T) - \|X - Y\|_F}, \tag{2.8}
\]
where we have used Weyl’s inequality \( |\sigma_m(X^T) - \sigma_m(Y^T)| \leq \|X - Y\|_F \) in the last step. To continue in (2.8), we have to estimate \( \|X - Y\|_F \) and \( \sigma_m(X^T) \).
We use the relation
\[
\left| \frac{\partial}{\partial e_j} f(x_k + \eta_{j,k} e_j) - \frac{\partial}{\partial e_j} f(x_k) \right| = \left| \sum_{i=1}^{m} [g'_i(a_i \cdot (x_k + \eta_{j,k} e_j)) - g'_i(a_i \cdot x_k)] a_{i,j} \right| \leq C \varepsilon \sum_{i=1}^{m} a_{i,j}^2
\]
to obtain the estimate
\[
\|X - Y\|_F = \|\mathcal{E}\|_F \leq C_2 \varepsilon \left( \sum_{k=1}^{m_X} \sum_{j=1}^{d} \left( \sum_{i=1}^{m} a_{i,j}^2 \right)^2 \right)^{1/2}
\]
(2.9)
\[
\leq C_2 \varepsilon \sqrt{m_X} \sum_{j=1}^{d} \sum_{i=1}^{m} a_{i,j}^2 = C_2 \varepsilon \sqrt{m_X} m.
\]
The statement now follows by a combination of (2.8) with (2.9) and (2.6).

**Remark 3.** The same argument as in the proof of Theorem 2.2 allows to show that
\[
\sigma_m(Y) - \sigma_{m+1}(Y) \geq \sqrt{m_X} (\sqrt{\alpha(1-s)} - 2C \varepsilon m)
\]
with the same probability as before. Hence, for \( \varepsilon \) small enough and \( m_X \) large, there is (with high probability) a gap in the spectrum of \( Y \) between \( \sigma_m(Y) \) and \( \sigma_{m+1}(Y) \). This can be used to detect \( m \) if it is unknown.

### 2.2.2 Passive sampling

In the previous sections we investigated the identification of the subspace \( A \) when the sample points of \( f(x) \) can be actively chosen. For that we used classical differentiation and Taylor’s residuals and we assumed exact evaluations of the function. In this section, we discuss the approximation of \( A \) in the more realistic scenario where the distribution of the sampling points is known, but not actively chosen, and the point evaluations are affected by noise.

As in [33], we assume that we are given a probability distribution \( \mu \), whose density \( p(x) \) is known or has been previously estimated from empirical data [19]. For simplicity we assume \( \text{supp}(p) \subset B^d \). We also assume that we are given a probability space \((\mathcal{V}, \pi)\) and a suitable collection of \( C^1_c \) functions \( \varphi_\nu : \mathbb{R}^d \to \mathbb{R} \), for \( \nu \in \mathcal{V} \), with the properties
\[
\text{supp} \varphi_\nu \subset B^d \text{ for all } \nu \in \mathcal{V}, \quad \max_{\nu \in \mathcal{V}} \max_{x \in B^d_1} \left\| \frac{\nabla \varphi_\nu(x)}{p(x)} \right\|_2 \leq C_\nu, \quad (2.10)
\]
and for which the matrix
\[
J_\mathcal{V}[f] = \int_{\mathcal{V}} \left( \int_{\mathbb{R}^d} \nabla f(x) \varphi_\nu(x) dx \right) \left( \int_{\mathbb{R}^d} \nabla f(x) \varphi_\nu(x) dx \right)^T d\pi(\nu) \quad (2.11)
\]
has full rank.

**Remark 4.** (i) The probability space \((\mathcal{V}, \pi)\), the set of functions \( \{ \varphi_\nu : \nu \in \mathcal{V} \} \), and the full-rank condition for \( J_\mathcal{V}[f] \) may appear abstract and a bit implicit at the first look. We clarify their role first in the most simple setting when \( m = 1, g(t) = t \) and \( \mathcal{V} = \{0\} \). Then \( f(x) = g(a \cdot x) = a \cdot x \) and (2.11) becomes
\[
J_\mathcal{V}[f] = a \cdot a^T \cdot \left( \int_{\mathbb{R}^n} \varphi_0(x) dx \right)^2
\]
It will turn out later (cf. Lemma 2.3 and Theorem 2.4), that we need to choose \( \varphi_0 : B^d_1 \rightarrow \mathbb{R} \), such that \( \alpha/C^2_\nu \) is as large as possible, where \( \alpha = \sigma_1(J_\nu[f]) \) stands for the spectral norm of \( J_\nu[f] \). Finally, if \( p(x) = \frac{1}{\omega_d} \) for every \( x \in B^d_1 \) with \( \omega_d \) denoting the Lebesgue volume of \( B^d_1 \) and \( \varphi_0 \) is radial with \( \varphi_0(1) = 0 \), we get

\[
\frac{\alpha}{C^2_\nu} = \frac{\left( I_{\mathbb{R}^n} \varphi_0(x)dx \right)^2}{\omega_d^2 \max_{x \in B_1^d} \| \nabla \varphi_0(x) \|^2_2} = \frac{\left( \int_{0}^{1} d\omega_d r^{d-1} \varphi_0(r)dr \right)^2}{\omega_d^2 \max_{0<r<1} |\varphi_0(r)|^2} \leq d^2 \left( \int_{0}^{1} \int_{r}^{1} ds \omega_d^{d-1} dr \right)^2 = d^2 \left( \int_{0}^{1} (1-r) r^{d-1} dr \right)^2 = d^2 \left( \frac{1}{d} - \frac{1}{d+1} \right)^2 = \frac{1}{(d+1)^2}.
\]

We observe that the conditions on \( \{ \varphi_\nu : \nu \in \mathcal{V} \} \) and \( J_\nu[f] \) may include an implicit dependence on \( d \). This is in accordance with the very well-known fact, that even the identification of one neuron (or one ridge function) can suffer the curse of dimension if we do not pose any additional restrictions on its activation function or its weights, cf. [5, 23, 42].

(ii) In fact, one may relate \((\mathcal{V}, \pi)\) and \( \{ \varphi_\nu : \nu \in \mathcal{V} \} \) directly to the density \( p \) as follows. We first consider a bounded resolution of the identity, i.e., a set of nonnegative smooth and compactly supported functions \( \psi_\nu \geq 0 \) such that \( \int_{\mathcal{V}} \psi_\nu(x) d\pi(\nu) = 1 \) for all \( x \in B^d_1 \) and \( \max_{\nu \in \mathcal{V}} \max_{x \in B_1^d} \| \nabla \psi_\nu(x) \|_2 \leq C_\Psi \). In case the set \( \mathcal{V} \) is discrete, then \( \{ \psi_\nu : \nu \in \mathcal{V} \} \) is simply a classical bounded partition of the unity. Additionally we pick yet another bounded and smooth function \( q \geq 0 \) such that \( \max_{x \in B_1^d} \| \psi_\nu(x) \|_2 \leq C_q \).

Then, one can define

\[
\varphi_\nu(x) = \psi_\nu(x) q(x),
\]

and it is not difficult to show that conditions (2.10) are fulfilled. In fact, for densities \( p \) with bounded derivatives, e.g., Gaussian mixtures, one could choose for instance \( q(x) = \frac{1}{2} p(x)^2 \). In fact, in this case, \( q(x)/p(x) = \frac{1}{2} p(x) \) and \( \nabla q(x)/p(x) = \nabla p(x) \).

Moreover, the matrix

\[
J_\nu[f] = \int_{\mathcal{V}} \left( \int_{\mathbb{R}^d} \nabla f(x) \psi_\nu(x) q(x) dx \right) \left( \int_{\mathbb{R}^d} \nabla f(x) \psi_\nu(x) q(x) dx \right)^T d\pi(\nu),
\]

would correspond to the superposition of “weighted local evaluations” of \( \nabla f \otimes \nabla f \) over the supports of the functions \( \psi_\nu \) to build a full-rank matrix.

Now, differently from [33], we consider the following empirical vectors

\[
Y_j = -\frac{1}{N} \sum_{k=1}^{N} \left( f(x_k) + n_k \right) \frac{\nabla \varphi_{\nu_j}(x_k)}{p(x_k)} \approx - \int_{\mathbb{R}^d} f(x) \frac{\nabla \varphi_{\nu_j}(x)}{p(x)} p(x) dx
\]

\[
= \int_{\mathbb{R}^d} \nabla f(x) \varphi_{\nu_j}(x) dx
\]

\[
= \sum_{i=1}^{m} \left( \int_{\mathbb{R}^d} g_i(x) \varphi_{\nu_j}(x) dx \right) a_i, \quad (2.12)
\]
generated at random by sampling i.i.d. \( \nu_j \sim \pi, j = 1, \ldots, m_X \). Here, the random variables \( n_k \) model the noise in the evaluation of the function \( f \) in the point \( x_k \) and we will assume that \( n_k \) are independent bounded centered random variables, i.e.,

\[
|n_k| \leq C_N \text{ with probability 1, and } E|n_k| = 0. \tag{2.13}
\]

The assumption that the noise is bounded can be relaxed to unbounded noise with thin tails (for instance sub-Gaussian noise) at the cost of adding in Theorem 2.4 below a negative term to the probability in the statement, which accounts for the probability that the noise realizations are in fact bounded. We define the matrix \( Y_{\nu} \in \mathbb{R}^{d \times m_N} \), whose columns are \( Y_j \), for \( j = 1, \ldots, m_X \). We similarly denote \( X_{\nu} \in \mathbb{R}^{d \times m_N} \) the matrix with columns \( X_j = \int_{\mathbb{R}^d} \nabla f(x) \varphi_{\nu_j}(x) dx \). With the same proof of Lemma 2.1 we can show the following result.

**Lemma 2.3.** Assume the vectors \((a_i)_{i=1}^m\) linearly independent, and \( \|a_i\|_2 = 1 \) for all \( i = 1, \ldots, m \). Additionally assume

\[
C_1 := \max_{i=1, \ldots, m} \max_{1 \leq t \leq 1} |g_i'(t)| < \infty.
\]

Suppose that \( \sigma_m(J_{\nu}[f]) \geq \alpha > 0 \), i.e., the \( m \)th singular value of the matrix \( J_{\nu}[f] \) is bounded away from zero. Then for any \( s \in (0, 1) \) we have that

\[
\sigma_m(X_{\nu}) \geq \sqrt{m \alpha (1 - s)}
\]

with probability at least \( 1 - m \exp\left(-\frac{m \alpha s^2}{2(C_0 C_N)}\right) \).

**Proof.** The only difference with respect to the proof of Lemma 2.1 is in how we estimate the term to the probability in the statement, which accounts for the probability that the noise (for instance sub-Gaussian noise) at the cost of adding in Theorem 2.4 below a negative term to the probability in the statement, which accounts for the probability that the noise realizations are in fact bounded. We define the matrix \( Y_{\nu} \in \mathbb{R}^{d \times m_N} \), whose columns are \( Y_j \), for \( j = 1, \ldots, m_X \). We similarly denote \( X_{\nu} \in \mathbb{R}^{d \times m_N} \) the matrix with columns \( X_j = \int_{\mathbb{R}^d} \nabla f(x) \varphi_{\nu_j}(x) dx \). With the same proof of Lemma 2.1 we can show the following result.

**Theorem 2.4.** Assume the vectors \((a_i)_{i=1}^m\) linearly independent, and \( \|a_i\|_2 = 1 \) for all \( i = 1, \ldots, m \). Additionally assume that

\[
C_\ell := \max_{i=1, \ldots, m} \max_{1 \leq t \leq 1} |g_i^{(\ell)}(t)| < \infty, \quad \ell = 0, 1.
\]

Let \( \tilde{A} \) be constructed as described in Algorithm 2.1 by substituting there \( Y \) with \( Y_{\nu} \), built by sampling N values of \( f \) as in (2.12). Let \( 0 < s < 1 \), and assume \( \sigma_m(J_{\nu}[f]) \geq \alpha > 0 \). Then

\[
\|P_A - P_{\tilde{A}}\|_F \leq \frac{2\eta}{\sqrt{\alpha(1 - s)} - \eta} \tag{2.15}
\]

with probability at least \( 1 - m \chi(d + 1) \exp\left(-\frac{s^2 N}{4(2(mQ)^2 + mQ^2/\eta)}\right) - m \exp\left(-\frac{m \alpha s^2}{2(mQ)^2}\right) \), where \( Q = (C_0 + C_N/m)C_N \). As a consequence, for any \( \varepsilon > 0 \) and \( \delta > 0 \),

\[
\|P_A - P_{\tilde{A}}\|_F \leq \varepsilon \tag{2.16}
\]

with probability at least \( 1 - \delta \) as soon as the number of sampling \( N \) values of \( f \) fulfills

\[
N \geq \frac{10(2 + \varepsilon)^2(mQ)^2}{\varepsilon^2 \alpha(1 - s)} \ln \left( \frac{4(d + 1)(mQ)^2 \ln(2m/\delta)}{\alpha s^2 \delta} \right) \tag{2.17}
\]

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Proof. As in the proof of Theorem 2.2

\[ \|P_A - P_{\bar{A}}\|_F \leq \frac{2\|X_Y - Y_V\|_F}{\sigma_m(X_Y^T)} - \|X_Y - Y_V\|_F. \]  \hspace{1cm} (2.18)

By Lemma 2.3 with probability at least \(1 - m \exp\left(-\frac{m^2 \alpha^2}{2(mQ)^2}\right)\) we have

\[ \sigma_m(X_V) \geq \sqrt{m\alpha(1-s)}. \]  \hspace{1cm} (2.19)

In order to conclude we need to estimate \(\|X_Y - Y_V\|_F\). We do it by applying Corollary 6.8 to estimate the quantity

\[ \|X_j - Y_j\|_2 = \left\| \frac{1}{N} \sum_{k=1}^{N} (f(x_k) + n_k) \frac{\nabla \varphi_{\nu}(x_k)}{p(x_k)} - \int_{\mathbb{R}^d} f(x) \frac{\nabla \varphi_{\nu}(x)}{p(x)} p(x) dx \right\|_2. \]

Let us denote \(X_{k,\nu} = (f(x_k) + n_k) \frac{\nabla \varphi_{\nu}(x_k)}{p(x_k)} - \int_{\mathbb{R}^d} f(x) \frac{\nabla \varphi_{\nu}(x)}{p(x)} p(x) dx\), which can be interpreted as a matrix of dimensions \(d \times 1\). We estimate its spectral norm or equivalently its \(\ell_2\)-norm as follows

\[ \|X_{k,\nu}\| = \left\| (f(x_k) + n_k) \frac{\nabla \varphi_{\nu}(x_k)}{p(x_k)} - \int_{\mathbb{R}^d} f(x) \frac{\nabla \varphi_{\nu}(x)}{p(x)} p(x) dx \right\|_2 \leq 2(mC_0 + C_N)C_V := K. \]

Moreover, we estimate

\[ \max \left\{ \left\| \frac{1}{N} \sum_{k=1}^{N} \mathbb{E}[X_{k,\nu}X_{k,\nu}^T] \right\|, \left\| \sum_{k=1}^{N} \mathbb{E}[X_{k,\nu}^T X_{k,\nu}] \right\| \right\} \leq \sum_{k=1}^{N} \mathbb{E}\|X_{k,\nu}\|^2 \]

\[ = \sum_{k=1}^{N} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left\| (f(y) + n) \frac{\nabla \varphi_{\nu}(y)}{p(y)} - \int_{\mathbb{R}^d} f(x) \frac{\nabla \varphi_{\nu}(x)}{p(x)} p(x) dx \right\|_2 p(y) dy d\omega(n) \]

\[ \leq NK^2 = N(2(mC_0 + C_N)C_V)^2 = \sigma^2, \]

where \(\omega\) is the probability distribution of the noise. Using \(K \leq 2mQ, \sigma^2 \leq 4N(mQ)^2\) and applying Corollary 6.8, we obtain

\[ \mathbb{P} \left( \left\| \frac{1}{N} \sum_{k=1}^{N} (f(x_k) + n_k) \frac{\nabla \varphi_{\nu}(x_k)}{p(x_k)} - \int_{\mathbb{R}^d} f(x) \frac{\nabla \varphi_{\nu}(x)}{p(x)} p(x) dx \right\|_2 > \eta \right) \]

\[ \leq (d + 1) \exp\left(-\frac{\eta^2 N}{4(2(mQ)^2 + mQ\eta/3)}\right). \]

By union bound over \(\nu_1, \ldots, \nu_{m\chi}\) we obtain

\[ \|X_Y - Y_V\|^2_F = \sum_{j=1}^{m\chi} \|X_j - Y_j\|^2_2 \leq m\chi \eta^2, \]  \hspace{1cm} (2.20)

with probability at least \(1 - m\chi(d + 1) \exp\left(-\frac{\eta^2 N}{4(2(mQ)^2 + mQ\eta/3)}\right)\). The proof of (2.15) is then obtained by combining (2.18), (2.19), and (2.20).
In order to show (2.16) and (2.17), let us fix \( \eta > 0 \) such that \( \varepsilon = \frac{2\eta}{\sqrt{\alpha(1-s)} - \eta} \), i.e.,

\[
\eta = \frac{\varepsilon \sqrt{\alpha(1-s)}}{2\varepsilon}.
\]

We now choose \( m_{X} \) large enough to ensure that

\[
\frac{\delta}{2} \geq m_{X} \exp\left(-\frac{m_{X}2^\alpha s^2}{2(mQ)^2}\right), \quad \text{i.e.} \quad m_{X} \geq \frac{2(mQ)^2 \ln(2m/\delta)}{\alpha s^2},
\]

and \( N \) large enough for

\[
\frac{\delta}{2} \geq (d + 1)m_{X} \exp\left(-\frac{\eta^2 N}{4(2(mQ)^2 + mQ\eta/3)}\right).
\]

Hence, using (2.14) and

\[
\frac{mQ}{\eta} \geq \frac{mC_{0}C_{Y}(2 + \varepsilon)}{\varepsilon \sqrt{\alpha(1-s)}} \geq \frac{mC_{0}C_{Y}}{\sqrt{\alpha}} \geq \frac{mC_{0}C_{Y}}{\sqrt{\sigma_{m}(J_{V}[f])}} \geq \frac{mC_{0}C_{Y}}{\sqrt{\sigma_{1}(J_{V}[f])}} \geq 1,
\]

we observe that for

\[
N \geq \frac{10(2 + \varepsilon)^2(mQ)^2}{\varepsilon^2 \alpha(1-s)} \ln\left(\frac{4(d + 1)(mQ)^2 \ln(2m/\delta)}{\alpha s^2 \delta}\right)
\]

we can ensure \( \|P_{A} - P_{\tilde{A}}\|_{F} \leq \varepsilon \), with probability at least \( 1 - \delta \).

3 Identification of network weights

We explained how to recover an approximation of \( A = \text{span}\{a_{1}, \ldots, a_{m}\} \) and how to use it to reduce the dimensionality of the problem from \( d \) to \( m \). We therefore concentrate on the case \( m = d \) in the rest of the paper.

We start to build the approximation scheme by approximating the ridge profiles. As we will show below, a crucial step in order to be able to identify/approximate the vectors \( a_{1}, \ldots, a_{m} \in \mathbb{R}^{m} \) is first to identify/approximate the span of their tensor products. Accordingly, we denote by

\[
\mathcal{A} = \text{span}\{a_{i} \otimes a_{i}, i = 1, \ldots, m\} \subset \mathbb{R}^{m \times m}
\]

the subspace of symmetric matrices generated by their tensor products \( a_{i} \otimes a_{i} = a_{i}a_{i}^{T} \). For the actual recovery of \( a_{i} \)'s we proceed according to the following strategy: we first recover an approximating subspace \( \tilde{\mathcal{A}} \) of symmetric matrices, which is (in some sense) close to \( \mathcal{A} \). Then, after a whitening process, which we explain in details in Section 3.3 below, we will be allowed to assume without loss of generality that the vectors \( a_{1}, \ldots, a_{m} \in \mathbb{R}^{m} \) are \( \varepsilon \)-nearly-orthonormal in the sense of Definition 1.1, i.e., that \( S(a_{1}, \ldots, a_{m}) \leq \varepsilon \) for \( \varepsilon > 0 \) small. (Some basic properties of this notion are collected in the Appendix for reader’s convenience and we refer to them below quite often.) Finally, we consider the following nonlinear program

\[
\text{arg max } \|M\|_{\infty}, \quad \text{s.t. } M \in \tilde{\mathcal{A}}, \|M\|_{F} \leq 1
\]

(3.1)

to recover the \( a_{i} \)'s - or, more precisely, their approximations \( \hat{a}_{i} \) (which is of course possible only up to the sign).

The optimization problem (3.1) is not convex and may in general have a large number of local maxima. Nevertheless, we shall prove that to every local maximizer of (3.1), there is one of the matrices \( a_{i} \otimes a_{i} \), which lies very close to it. In particular, for \( \tilde{\mathcal{A}} = \mathcal{A} \) and the vectors \( a_{1}, \ldots, a_{m} \in \mathbb{R}^{m} \) orthonormal, we obtain the exact recovery of the \( a_{i} \otimes a_{i} \)'s.
3.1 Approximation of $\mathcal{A}$

First of all we construct here an approximation $\tilde{\mathcal{A}}$ to the space $\mathcal{A} = \text{span}\{a_i \otimes a_i, i = 1, \ldots, m\}$. As in the previous sections we describe two different methods of identification of $\mathcal{A}$. The first one is by active sampling and makes use of second order differences. The second one implements passive sampling under the assumption that we dispose of the probability density $p(x)$ of the point distribution.

3.1.1 Active sampling

We start by generating again $mX \in N$ points $x_l \sim \mu_{S^{m-1}}, l = 1, \ldots, m$ uniformly at random on the $m-1$ dimensional sphere (remind that now we assume $m = d$), and we define

$$(\Delta[f](x_l))_{j,k} = \frac{f(x_l + \epsilon (e_j + e_k)) - f(x_l + \epsilon e_j) - f(x_l + \epsilon e_k) + f(x_l)}{\epsilon^2}, \quad j, k = 1, \ldots, m.$$  

As $\Delta[f](x) \sim \nabla^2 f(x) = \sum_{i=1}^m g''_i(a_i \cdot x)a_i a_i^T \in \mathcal{A}$, we define $\tilde{\mathcal{A}}$ as the $m$-dimensional subspace approximating the points $(\Delta[f](x_l))_{l=1}^{mX}$ in the least-square sense. For later use we define $Y$ the $m^2 \times mX$ matrix with columns vec($\Delta[f](x_l)$), i.e.,

$$Y = (\text{vec}(\Delta[f](x_1))| \ldots | \text{vec}(\Delta[f](x_{mX}))). \quad (3.2)$$

We show below that $\tilde{\mathcal{A}}$ is indeed a good approximation to $\mathcal{A}$ by showing that the difference of the respective orthogonal projections $\|P_{\mathcal{A}} - P_{\tilde{\mathcal{A}}}\|_F$ in the operator norm associated to the Frobenius norm of matrices is small with high probability, as soon as $mX$ is large enough.

We need now to introduce some notations to facilitate the presentation. We define the vectorization of a matrix $A = (a_{i,j})_{ij} \in \mathbb{R}^{m \times m}$ as the column vector in $\mathbb{R}^{m^2}$

$$\text{vec}(A)_k := a_{\left\lfloor \frac{k-1}{m} \right\rfloor + 1, (k-1 \mod m) + 1}, \quad k = 1, \ldots, m^2.$$  

For two matrices $A, B \in \mathbb{R}^{m \times m}$ we define their vectorized tensor product by

$$A \otimes_v B := \text{vec}(A) \otimes \text{vec}(B) = \text{vec}(A) \text{vec}(B)^T. \quad (3.3)$$

(Note that such a product of matrices does coincide neither with the Hadamard product nor with the Kronecker product.) Thanks to these definitions and notations we can introduce the matrix

$$H_2[f] := \int_{S^{m-1}} \nabla^2 f(x) \otimes_v \nabla^2 f(x) d\mu_{S^{m-1}}(x).$$

This $m^2 \times m^2$ matrix plays exactly the same role as $J[f]$ in Section 2.2.1.
**Algorithm 3.1.**

- Construct $Y$ as in (3.2).
- Compute the singular value decomposition of

\[
    Y^T = \begin{pmatrix} \tilde{U}_1 & \tilde{U}_2 \end{pmatrix} \begin{pmatrix} \tilde{\Sigma}_1 & 0 \\ 0 & \tilde{\Sigma}_2 \end{pmatrix} \begin{pmatrix} \tilde{V}_1^T \\ \tilde{V}_2^T \end{pmatrix},
\]

where $\tilde{\Sigma}_1$ contains the $m$ largest singular values.
- Set $\tilde{A}$ to be the space of matrices, whose vectorization lies in the row space of $\tilde{V}_1^T$.

As we follow the same strategy as the one used in Section 2.2.1 to approximate the space $A = \text{span}\{a_i, i = 1, \ldots, m\}$, we limit ourselves to reformulate it in the context of the vector space of matrices $A$. We start with a technical estimate, which is essentially based on Taylor’s theorem.

**Lemma 3.1.** Assume the vectors $(a_i)_{i=1}^m$ satisfy $\|a_i\|_2 = 1$ for all $i = 1, \ldots, m$ and assume that $g_j, j = 1, \ldots, m$, are two times differentiable with the Lipschitz constant of all $g_j''$, $j = 1, \ldots, m$ bounded from above by $C_3 > 0$. Then, for all $x \in \mathbb{S}^{m-1}$,

\[
    \|\nabla^2 f(x) - \Delta[f](x)\|_F \leq 2C_3m\epsilon.
\]

**Proof.** Let $g(t) = f(x + te_j + \epsilon e_k) - f(x + te_j)$, where $0 \leq t \leq \epsilon$. Then by the mean value theorem

\[
    (\Delta[f](x))_{j,k} = \frac{g(\epsilon) - g(0)}{\epsilon^2} = \frac{g'(\xi_1)}{\epsilon} = \frac{\partial f}{\partial x_j}(x + \xi_1 e_j + \epsilon e_k) - \frac{\partial f}{\partial x_j}(x + \xi_1 e_j)
\]

\[
    = \frac{\partial^2 f}{\partial x_k \partial x_j}(x + \xi_1 e_j + \xi_2 e_k),
\]

where $0 < \xi_1, \xi_2 < \epsilon$. Therefore

\[
    |(\nabla^2 f(x))_{j,k} - (\Delta[f](x))_{j,k}| = \left| \frac{\partial^2 f}{\partial x_k \partial x_j}(x) - \frac{\partial^2 f}{\partial x_k \partial x_j}(x + \xi_1 e_j + \xi_2 e_k) \right|
\]

\[
    \leq \sum_{l=1}^m |g''(a_l \cdot x) - g''(a_l \cdot (x + \xi_1 e_j + \xi_2 e_k))| |a_{l,j}| |a_{i,k}|
\]

\[
    \leq C_3 \epsilon \sum_{l=1}^m |a_{l,j}| |a_{i,k}| (|a_{l,j}| + |a_{i,k}|).
\]

Using triangle inequality and $\|a_j\|_4 \leq \|a_j\|_2 = 1$, we estimate

\[
    \|\nabla^2 f(x) - \Delta[f](x)\|_F \leq 2C_3 \epsilon \left[ \sum_{j,k=1}^m \left( \sum_{i=1}^m a_{i,j}^2 |a_{i,k}| \right)^2 \right]^{1/2} \leq 2C_3 \epsilon \sum_{i=1}^m \left( \sum_{j,k=1}^m a_{i,j}^4 a_{i,k}^2 \right)^{1/2}
\]

\[
    = 2C_3 \epsilon \sum_{i=1}^m \left( \sum_{j=1}^m a_{i,j}^4 \right)^{1/2} \left( \sum_{k=1}^m a_{i,k}^2 \right)^{1/2} \leq 2C_3 \epsilon m.
\]

\[\Box\]
Theorem 3.2. Assume the vectors \((a_i)_{i=1}^m\) linearly independent, and \(\|a_i\|_2 = 1\) for all \(i = 1, \ldots, m\). Additionally assume
\[
C_j := \max_{i=1,\ldots,m} \max_{1\leq t \leq 1} |g_i^{(j)}(t)| < \infty, \quad j = 0, 1, 2.
\]
Let \(\tilde{A}\) be constructed as described in Algorithm 3.1 by sampling \(m\chi [(m + 1)(m + 2)/2]\) values of \(f\). Let \(0 < s < 1\), and assume \(\sigma_m(H_2[f]) \geq \alpha_2 > 0\), i.e., the \(m\)th singular value of the matrix \(H_2[f]\) is bounded away from zero. Then
\[
\|\hat{P}_A - P_{\tilde{A}}\|_{F \to F} \leq \frac{4C_3\epsilon m}{\sqrt{\alpha_2 (1 - s)} - 2C_3\epsilon m}
\]
with probability at least \(1 - m \exp \left( - \frac{m\chi \alpha_2^2}{2mC_2^2} \right)\). In particular \(\dim(A) = \dim(\tilde{A}) = m\).

Proof. We define the matrices \(X, Y\) whose columns are given by \(\text{vec}(\nabla^2 f(x_j)), j = 1, \ldots, m\chi\) and \(\text{vec}(\Delta[f](x_j)), j = 1, \ldots, m\chi\) respectively, namely
\[
X = (\text{vec}(\nabla^2 f(x_1))) \ldots (\text{vec}(\nabla^2 f(x_{m\chi}))), \quad Y = (\text{vec}(\Delta[f](x_1))) \ldots (\text{vec}(\Delta[f](x_{m\chi}))).
\]
Notice that these matrices have dimension \(m^2 \times m\chi\). As done in (2.8) and by assuming for the moment that \(\sigma_m(X) \neq 0\) (but obviously \(\sigma_{m+1}(X) = 0\) because the \(\nabla^2 f(x_i)\)'s lie all in the \(m\)-dimensional space \(A\)), we deduce the estimate
\[
\|\hat{P}_A - P_{\tilde{A}}\|_{F \to F} \leq \frac{2\|X - Y\|_F}{\sigma_m(X) - \|X - Y\|_F}, \quad (3.4)
\]
as an application of Wedin’s bound, Theorem 6.6 in the Appendix. From Lemma 3.1 we easily deduce
\[
\|X - Y\|_F = \left( \sum_{j=1}^{m\chi} \|\nabla^2 f(x_j) - \Delta[f](x_j)\|_F^2 \right)^{1/2} \leq 2C_3\epsilon m \sqrt{m\chi}. \quad (3.5)
\]
In order to apply (3.4) we need finally to estimate \(\sigma_m(X)\) from below and we shall do it by using again the Chernoff’s bound for matrices Theorem 6.7.

Given an orthonormal basis \(\{B_1, \ldots, B_m\}\) for \(A\) we define the projector from \(\mathbb{R}^{m^2} \to \mathbb{R}^m\) given by \(P^A v = (\text{vec}(B_1)^T v, \ldots, (\text{vec}(B_m)^T v)\) for any \(v \in \mathbb{R}^{m^2}\). We additionally define with some abuse of notation
\[
P^A X := (P^A(\text{vec}(\nabla^2 f(x_1))) \ldots (P^A(\text{vec}(\nabla^2 f(x_{m\chi}))))).
\]
Notice that now this matrix has dimension \(m \times m\chi\). Thanks to the fact that \(P^A\) is an orthogonal transformation, we obtain the following equivalences
\[
\sigma_m(X) = \sqrt{\sigma_m((P^A X)(P^A X)^T)}.
\]
Hence to estimate \(\sigma_m(X)\), it is sufficient to do it for \(\sigma_m((P^A X)(P^A X)^T)\), whose argument is explicitly expressed as a sum
\[
(P^A X)(P^A X)^T = \sum_{j=1}^{m\chi} X_j,
\]
where
where
\[ X_j = P^A \text{vec}(\nabla^2 f(x_j)) \otimes \text{vec}(\nabla^2 f(x_j))(P^A)^T. \]

We wish to apply Theorem 6.7 for the sequence of positive semidefinite matrices \( X_1, \ldots, X_m \).

We notice first that
\[ \mathbb{E}X_j = P^A H^f_j (P^A)^T, \]
and therefore
\[ \mu \min(\mathbb{E}X_j) \geq m^\chi \alpha_2. \quad (3.6) \]

Additionally, for every \( x \in S^{m-1} \)
\[ \sigma_1(P^A \text{vec}(\nabla^2 f(x)) \otimes_v \text{vec}(\nabla^2 f(x))(P^A)^T) = \sigma_1(\text{vec}(\nabla^2 f(x)) \otimes_v \text{vec}(\nabla^2 f(x))) \leq \|\nabla^2 f(x_j)\|^2_F \]
\[ = \| \sum_{i=1}^m g''(a_i \cdot x) a_i \otimes a_i \|^2_F \leq C_2^2 m^2. \]

An application of Theorem 6.7 under conditions (3.6) and (3.7) yields
\[ \sigma_m(X) \geq \sqrt{m^\chi \alpha_2(1 - s)}, \quad (3.7) \]
with probability
\[ 1 - m \exp \left( -\frac{m^\chi \alpha_2 s^2}{2m^2 C_2^2} \right). \]

We conclude from (3.5) and (3.7) that, with the same probability
\[ \| P_A - P_{\tilde{A}} \|_{F \rightarrow F} \leq \frac{4C_3 m \epsilon}{\sqrt{\alpha_2(1 - s) - 2C_3 m \epsilon}}. \]

3.1.2 Passive sampling

We again assume that we are given a probability space \((V, \pi)\) and a suitable collection of \( C^2_\nu \) functions \( \varphi_\nu : \mathbb{R}^d \rightarrow \mathbb{R} \), for \( \nu \in V \), with the properties
\[ \text{supp} \varphi_\nu \subset B_1^d \text{ for all } \nu \in V, \quad \max_{\nu \in V} \max_{x \in B_1^d} \left\{ \int_{\mathbb{R}^d} |\varphi_\nu(x)| dx, \max_{x \in B_1^d} \frac{\| \nabla^2 \varphi_\nu(x) \|}{p(x)} \right\} \leq C_\nu 2, \]
where in the latter bound we consider the spectral norm. Furthermore, we also assume that the matrix
\[ H_V[f] = \int_V \left( \int_{\mathbb{R}^d} \nabla^2 f(x) \varphi_\nu(x) dx \right) \otimes_v \left( \int_{\mathbb{R}^d} \nabla^2 f(x) \varphi_\nu(x) dx \right)^T d\pi(\nu) \]
has full rank. We consider the following empirical vectors
\[ Y_j = \text{vec} \left( \frac{1}{N} \sum_{k=1}^N \left( f(x_k) + n_k \right) \frac{\nabla^2 \varphi_{\nu_j}(x_k)}{p(x_k)} \right) \approx \text{vec} \left( \int_{\mathbb{R}^d} f(x) \frac{\nabla^2 \varphi_{\nu_j}(x)}{p(x)} p(x) dx \right) \]
\[ = \text{vec} \left( \int_{\mathbb{R}^d} \nabla^2 f(x) \varphi_{\nu_j}(x) dx \right) \]
\[ = \sum_{i=1}^m \text{vec} \left( \left( \int_{\mathbb{R}^d} g''(a_i \cdot x) \varphi_{\nu_j}(x) dx \right) a_i \otimes a_i \right), \quad (3.8) \]

\[ 23 \]
generated at random by sampling i.i.d. $\nu_j \sim \pi$, $j = 1, \ldots, m_X$, for $m_k$ independent random bounded and centered noise fulfilling (2.13). We define the matrix $Y_{\nu,2} \in \mathbb{R}^{m \times m_X}$, whose columns are $Y_j$, for $j = 1, \ldots, m_X$. We similarly denote $X_{\nu,2} \in \mathbb{R}^{m \times m_X}$ the matrix with columns $X_j = \text{vec} \left( \int_{\mathbb{R}^d} \nabla^2 f(x) \varphi_{\nu_j}(x) dx \right)$.

Then, by an analogous proof as for Theorem 3.2 and Theorem 2.4, and again applications of Theorem 6.7 and Corollary 6.8 we obtain the following result.

**Theorem 3.3.** Assume the vectors $(a_i)_{i=1}^m$ linearly independent, and $\|a_i\|_2 = 1$ for all $i = 1, \ldots, m$. Additionally assume

$$C_j := \max_{i=1,\ldots,m} \max_{-1 \leq t \leq 1} |g_{ij}(t)| < \infty, \quad j = 0, 1, 2.$$ 

Let $\tilde{A}$ be constructed as described in Algorithm 3.1 by substituting there $Y$ with $Y_{\nu,2}$, built by sampling $N$ values of $f$ as in (3.8). Let $0 < s < 1$, and assume $\sigma_m(H_{Y}[f]) \geq \alpha_2 > 0$. Then

$$\|P_{\tilde{A}} - P_A\|_{F \rightarrow F} \leq \frac{2\eta}{\sqrt{\alpha_2(1-s)} - \eta}$$

with probability at least $1 - \frac{2m\alpha_2}{\eta^2 N} \exp \left( - \frac{\eta^2 N}{2(2m\alpha_2)^2} \right)$, for $Q = (\max\{C_0, C_2\} + C_X/m)C_{\nu,2}$. As a consequence, for any $\varepsilon > 0$ and $\delta > 0$,

$$\|P_{\tilde{A}} - P_A\|_{F \rightarrow F} \leq \varepsilon,$$

with probability at least $1 - \delta$ as soon as the number of sampling $N$ values of $f$ fulfills

$$N \geq \frac{10(2 + \varepsilon)^2(mQ)^2}{\varepsilon^2 \alpha_2(1-s)} \ln \left( \frac{8m^3 Q^2 \ln(2m/\delta)}{\alpha_2^2 \delta} \right).$$

**Proof.** By Wedin’s bound, we obtain as in the proof of Theorem 2.4

$$\|P_{\tilde{A}} - P_A\|_{F \rightarrow F} \leq \frac{2\|X_{\nu,2} - Y_{\nu,2}\|_F}{\sigma_m(X_{\nu,2}^T) - \|X_{\nu,2} - Y_{\nu,2}\|_F}.$$ 

The analogue of (2.7) and (2.14) now reads as

$$\sigma_1 \left( P_A \left( \int_{\mathbb{R}^d} f(x) \nabla^2 \varphi_{\nu}(x) \frac{p(x)}{p(x)} dx \right) \otimes_v \left( \int_{\mathbb{R}^d} f(x) \nabla^2 \varphi_{\nu}(x) \frac{p(x)}{p(x)} dx \right)^T \right) \leq \int_{\mathbb{R}^d} \nabla^2 f(x) \varphi_{\nu}(x) dx = \sum_{i=1}^m \int_{\mathbb{R}^d} g_i''(a_i \cdot x) \varphi_{\nu}(x) dx \left( a_i \otimes a_i \right) \leq (C_2C_Ym)^2.$$

Then for any $s \in (0,1)$ we have that

$$\sigma_m(X_{\nu,2}) \geq \sqrt{m\alpha_2(1-s)}$$

with probability at least $1 - m \exp \left( \frac{-m\alpha_2}{2(C_2C_Ym)^2} \right)$.

Let us denote $X_{k,\nu} = (f(x_k) + n_k) \nabla^2 \varphi_{\nu}(x_k) / p(x_k) - \int_{\mathbb{R}^d} f(x) \nabla^2 \varphi_{\nu}(x) \frac{p(x)}{p(x)} dx$, which is a matrix of dimensions $m \times m$. We estimate its spectral norm by $\|X_{k,\nu}\| \leq 2(mC_0 + C_N)C_{\nu,2} = K$. 24
Moreover, we estimate
\[
\max \left\{ \left\| \sum_{k=1}^{N} E[X_{k,\nu}X_{k,\nu}^T] \right\|, \left\| \sum_{k=1}^{N} E[X_{k,\nu}X_{k,\nu}^T] \right\| \right\} \leq \sum_{k=1}^{N} E\left[\|X_{k,\nu}\|^2\right]
\]
\[
\leq \sum_{k=1}^{N} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left| (f(y) + n) \nabla^2 \varphi_{y}(y) p(y) - \int_{\mathbb{R}^d} f(x) \nabla^2 \varphi_{x}(x) p(x) dx \right|^2 p(y) dy d\omega(n)
\]
\[
\leq N(2(mC_0 + C_V)C_V)^2 := \sigma^2,
\]
where \( \omega \) is the probability distribution of the noise. Hence, by an application of Corollary 6.8
\[
P\left(\|X_j - Y_j\|_2 > \eta\right) = P\left(\left\| \frac{1}{N} \sum_{k=1}^{N} X_{k,\nu} \right\|_F > \eta\right) \leq 2m \exp\left(-\frac{\eta^2 N}{4(2mQ)^2 + mQ\eta/3}\right).
\]
To estimate \( \|X_{V,2} - Y_{V,2}\|_F \), we use the union bound over \( \nu_1, \ldots, \nu_m, x \) and obtain that
\[
\|X_{V,2} - Y_{V,2}\|_F^2 = \sum_{j=1}^{m} \|X_j - Y_j\|_2^2 \leq m\chi \eta^2, \tag{3.14}
\]
with probability at least \( 1 - 2mm\chi \exp\left(-\frac{\eta^2 N}{4(2mQ)^2 + mQ\eta/3}\right) \). The final bound then follows by combining (3.12), (3.13), and (3.14).

The proof of (3.10) and (3.11) proceeds in the same manner as in the proof of Theorem 2.4. \( \square \)

3.2 Properties of local maximizers

In this section we return to the analysis of the optimization program (3.1), i.e.
\[
\text{arg max } \|M\|_{\infty}, \quad \text{s.t. } M \in \tilde{A}, \quad \|M\|_F \leq 1, \tag{3.15}
\]
and we derive a characterization of its local maximal solutions. First of all let us observe that every local maximizer of (3.15) will be always found on the sphere \( \mathbb{S}_{\tilde{A}} = \{ M \in \tilde{A} : \|M\|_F = 1 \} \). The set \( \mathbb{S}_{\tilde{A}} \) is a unit sphere in a Hilbert space of (symmetric) matrices, intersected with a linear subspace, and therefore everywhere differentiable. Despite the nonsmoothness of the objective function, i.e. \( M \to \|M\|_{\infty} \), the solution of the nonconvex program (3.15) will be tackled by means of differential methods.

Our general approach is the following. Let us assume, that \( M \) is a local maximizer of (3.15), then there is a neighborhood \( \mathcal{U} \subset \mathbb{S}_{\tilde{A}} \) of \( M \) on the sphere \( \mathbb{S}_{\tilde{A}} \), such that \( \|X\|_{\infty} \leq \|M\|_{\infty} \) for every \( X \in \mathcal{U} \). Hence for every \( X \in \tilde{A} \), the function
\[
f_X : \gamma \to \frac{\|M + \gamma X\|_{\infty}}{\|M + \gamma X\|_F} \tag{3.16}
\]
has a local maximum in \( \gamma = 0 \). Furthermore, without loss of generality it is enough to restrict ourselves to matrices \( X \in \tilde{A} \) with \( \|X\|_F = 1 \) and \( X \perp M \) (in the scalar product \( \langle \cdot, \cdot \rangle_F \) induced by the Frobenius norm). In fact, by considering any \( X = \alpha M + X_{\perp} \) with \( X_{\perp} \perp M \) we have
\[
f_X(\gamma) = \frac{\|M + \gamma(\alpha M + X_{\perp})\|_{\infty}}{\|M + \gamma(\alpha M + X_{\perp})\|_F} = \frac{\|M + \gamma/(1 + \gamma \alpha)X_{\perp}\|_{\infty}}{\|M + \gamma/(1 + \gamma \alpha)X_{\perp}\|_F} = f_{X_{\perp}}(\gamma/(1 + \gamma \alpha)).
\]
Let now
\[(M + \gamma X)u_j(\gamma) = \lambda_j(\gamma)u_j(\gamma), \quad j = 1, \ldots, m,\] (3.17)
be the spectral decomposition of \(M + \gamma X\) with eigenvalues \(\lambda_j(\gamma)\) and eigenvectors \(u_j(\gamma)\). For the sake of a simple introduction to the characterization result (we provide of it below a more formal proof), let us assume just for now that \(\lambda_j(\gamma)\) and \(u_j(\gamma)\) depend smoothly on \(\gamma\). For \(\gamma = 0\), we denote briefly \(u_j = u_j(0)\) and \(\lambda_j = \lambda_j(0)\) and (3.17) becomes \(Mu_j = \lambda_ju_j\).

Due to \(\|M + \gamma X\|_{p^{-1}} = (1 + \gamma^2)^{-1/2} = 1 - \gamma^2/2 + o(\gamma^2)\), we obtain asymptotically for \(\gamma \to 0\)
\[f_X(\gamma) = (1 - \gamma^2/2) \cdot \max_{j:|\lambda_j(0)| = \|M\|_\infty} |\lambda_j(0) + \lambda_j'(0)\gamma + \lambda_j''(0)\gamma^2/2| + o(\gamma^2).\] (3.18)

We conclude, that if \(f_X\) has a local maximum in \(\gamma = 0\), then, by a simple asymptotic argument for \(\gamma \to 0\), we conclude
\[\lambda_j'(0) = 0,\] (3.19)
for all \(j \in \{1, \ldots, m\}\) with \(|\lambda_j(0)| = \|M\|_\infty\).

In order to determine \(\lambda_j'(0)\), we differentiate (3.17)
\[Mu_j' = Xu_j + \gamma Xu_j' = \lambda_j u_j + \lambda_j(u_j' + \gamma u_j),\] (3.20)
evaluate (3.20) in \(\gamma = 0\) and multiply it with \(u_j\). We obtain
\[(u_j^T)^2 Mu_j + u_j^T Xu_j = \lambda_j^2(0) + \lambda_j u_j^T u_j'.\]

We now plug in the relation \(Mu_j = \lambda_j u_j\) together with \((u_j)^T u_j = 0\), which follows by differentiating the orthogonality relation \(\langle u_i(\gamma), u_j(\gamma)\rangle = \delta_{i,j}\), and obtain
\[\lambda_j'(0) = u_j^T Xu_j.\]

In view of (3.19), we have in particular
\[0 = u_j^T Xu_j,\]
for all \(j \in \{1, \ldots, m\}\) with \(|\lambda_j(0)| = \|M\|_\infty\). The latter equations are actually the first order optimality conditions for \(M\) being an extremal point for (3.15).

To distinguish between local minimizers and local maximizers, we study also the second derivatives. Again for the sake of simplicity, we assume now that the largest eigenvalue of \(M\) is simple (below we actually prove this property). As we can always exchange \(M\) with \(-M\), we shall assume in the sequel that \(\lambda_1 = \|M\|_\infty > \max\{\lambda_2, \ldots, \lambda_m\}\). In this case we reformulate (3.18) using \(\lambda_1'(0) = 0\) and (3.18) becomes
\[f_X(\gamma) = (1 - \gamma^2/2)(\lambda_1(0) + \lambda_1''(0)\gamma^2/2) + o(\gamma^2) = \lambda_1(0) + \frac{\lambda_1''(0) - \lambda_1(0)}{2} \gamma^2 + o(\gamma^2).\]

If \(f_X\) has a local maximum at \(\gamma = 0\), again by a simple asymptotic argument for \(\gamma \to 0\), we conclude that
\[\lambda_1''(0) \leq \lambda_1(0).\] (3.21)

We differentiate (3.20) with \(j = 1\) to obtain
\[Mu_1'' + 2Xu_1' + \gamma Xu_1' = \lambda_1''u_1 + 2\lambda_1'u_1' + \lambda_1u_1'.\]
We evaluate this equation at $\gamma = 0$ and take again the inner product with $u_1$, yielding

$$u_1^T M u_1'' + 2u_1^T X u_1' = \lambda_1''(0) + 2\lambda_1'(0)u_1^T u_1' + \lambda_1 u_1^T u_1''.$$  
Using $u_1^T M u_1'' = \lambda_1 u_1^T u_1''$ and $u_1^T u_1' = 0$, the equation becomes

$$\lambda_1''(0) = 2u_1^T X u_1'.$$

For eliminating $u_1'$, we multiply (3.20) for $j = 1$ with $u_k, k \neq 1$ at $\gamma = 0$. This gives

$$u_k^T M u_1' + u_k^T X u_1 = \lambda_1'(0)u_k^T u_1 + \lambda_1 u_k^T u_1'.$$

Using $u_k^T M u_1' = \lambda_k u_k^T u_1'$ and $u_k^T u_1 = 0$, this can be reformulated as $u_k^T u_1' = (u_k^T X u_1)/(\lambda_1 - \lambda_k)$ for $\lambda_1 \neq \lambda_k$. Hence

$$u_1' = \sum_{k=1}^{m} \langle u_1', u_k \rangle u_k = \sum_{k=2}^{m} \frac{(u_k^T X u_1)}{\lambda_1 - \lambda_k} u_k$$

and (3.21) becomes

$$2u_1^T X \left( \sum_{k=2}^{m} \frac{u_k^T X u_k}{\lambda_1 - \lambda_k} u_k \right) = 2 \sum_{k=2}^{m} \frac{(u_1^T X u_k)^2}{\lambda_1 - \lambda_k} \leq \lambda_1$$

for all $X \in S_{\tilde{A}}$ with $X \perp M$. The equation (3.22) corresponds to the second order optimality condition for $M$ being a local maximizer for (3.15).

In the argument above we made heavy use of the additional requirement of smooth dependence of the spectral decomposition of $M + \gamma X$ on the parameter $\gamma$. We will show now, that the same is true even without such an assumption.

**Theorem 3.4.** Let $M$ be any local maximizer of

$$\arg \max \|M\|_{\infty}, \quad \text{s.t.} \quad M \in \tilde{A}, \quad \|M\|_F \leq 1.$$  

Then

$$u_j^T X u_j = 0 \quad \text{for all} \quad X \in S_{\tilde{A}} \quad \text{with} \quad X \perp M$$

and all $j \in \{1, \ldots, m\}$ with $|\lambda_j(0)| = \|M\|_{\infty}$.

If furthermore

$$S(a_1, \ldots, a_m) \leq \varepsilon \quad \text{and} \quad 3m\|P_A - P_{\tilde{A}}\| < (1 - \varepsilon)^2,$$

then $|\lambda_1| = \|M\|_{\infty}$, $\lambda_1 \notin \{\lambda_2, \ldots, \lambda_m\}$ and

$$2 \sum_{k=2}^{m} \frac{(u_1^T X u_k)^2}{|\lambda_1 - \lambda_k|} \leq |\lambda_1| \quad \text{for all} \quad X \in S_{\tilde{A}} \quad \text{with} \quad X \perp M.$$  

Before presenting the proof of this result let us add some comments on the orthogonality condition $X \perp M$.  

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Remark 5. (i) If $X \in \tilde{A}$ is not orthogonal to $M$, we consider the matrix

$$
\frac{X - (X, M)M}{\|X - (X, M)M\|_F}
$$

for every $X \in \tilde{A}$ not co-linear with $M$, and can rewrite (3.24) as

$$
u_j^T Xu_j = \langle X, M \rangle \|M\|_\infty \quad \text{for every } X \in \tilde{A},
$$

(3.27)

for all $j \in \{1, \ldots, m\}$ with $|\lambda_j(0)| = \|M\|_\infty$. Moreover, if $X$ is a multiple of $M$, this relation holds trivially. Furthermore (3.26) becomes

$$
2 \sum_{k=2}^m \frac{(u_k^T Xu_k)^2}{\lambda_1 - \lambda_k} \leq \|M\|_\infty \cdot \|X - (X, M)M\|_F^2
$$

(3.28)

for all $X \in \tilde{A}$; again, if $X$ is a multiple of $M$, this relation is trivial.

(ii) The formulas (3.24) and (3.26) resemble very much the so-called first and second Hadamard variation formula, cf. [62, Chapter 1.3]. At least in the case when the spectrum of $M$ contains only simple eigenvalues, the proof we give resembles very much the one in [62].

Proof of Theorem 3.4.

Step 1. Proof of (3.24)

Let us assume, that $M \in \tilde{A}$ is fixed and that $f_X$ has local maximum at $\gamma = 0$ for $X \in \tilde{A}$ with $\|X\|_F = 1$ and $X \perp M$. Hence, for $|\gamma|$ small, we have

$$
\|M\|_\infty \geq \|M + \gamma X\|_\infty \geq \left(1 - \gamma^2/2 + o(\gamma^2)\right) \cdot \max_{j=1,\ldots,m} |u_j^T (M + \gamma X)u_j|
$$

$$
= \max_{j=1,\ldots,m} \left|\lambda_j(0) + \gamma u_j^T Xu_j\right| + O(\gamma^2).
$$

Considering $j \in \{1, \ldots, m\}$ with $|\lambda_j(0)| = \|M\|_\infty$ and $|\gamma|$ small, we arrive to (3.24).

Step 2. Proof of (3.26)

We derive (3.26) under the assumption that $\lambda_1 = \|M\|_\infty$ and $\lambda_1 \notin \{\lambda_2, \ldots, \lambda_m\}$. If $\lambda_1 = -\|M\|_\infty$, the result follows by considering $-M$ instead of $M$.

Let again $Mu_j = \lambda_j u_j$ be the singular value decomposition of $M$. Then

$$
\|M + \gamma X\|_\infty \geq \left(\sum_{i=1}^m \sigma_i^2 u_i\right)^T (M + \gamma X) (\sum_{j=1}^m \sigma_j u_j)
$$

$$
= \max_{\|\sigma\|_2 \leq 1} \left(\sum_{i,j=1}^m \sigma_i \sigma_j u_i^T Mu_j + \gamma \sum_{i,j=1}^m \sigma_i \sigma_j u_i^T Xu_j\right)
$$

(3.29)

$$
= \max_{\|\sigma\|_2 \leq 1} \left(\sum_{i=1}^m \sigma_i^2 \lambda_i + \gamma \sum_{i,j=1}^m \sigma_i \sigma_j A_{ij}\right) =: \sup_{\|\sigma\|_2 \leq 1} f(\sigma),
$$

where $A_{ij} = u_i^T Xu_j = A_{ji}$. We will use an approximate solution of the Lagrange’s multiplier equations to estimate $\|M + \gamma X\|_\infty$ from below.
We set the constraint condition $g(\sigma) = \|\sigma\|_2^2 = 1$ and use Lagrange’s multiplier theorem on 
\[ \theta(\sigma, \nu) := f(\sigma) + \nu(g(\sigma) - 1). \]

This leads to equations 
\[ \frac{\partial \theta}{\partial \nu} = g(\sigma) - 1 = 0, \]
\[ \frac{\partial \theta}{\partial \sigma_j} = 2\sigma_j \lambda_j + 2\gamma \sum_{i=1}^{m} \sigma_i A_{ij} + \nu \cdot 2\sigma_j = 0, \quad j = 1, \ldots, m. \quad (3.30) \]

For $j = 1$ we use $A_{11} = u_1^T X u_1 = 0$ and (3.30) becomes 
\[ \sigma_1 (\lambda_1 + \nu) = -\gamma \sum_{j=2}^{m} \sigma_j A_{1j}. \quad (3.31) \]

If $j \geq 2$, we reduce (3.30) by the following observation. The optimal value of $\sigma$ in (3.29) for $\gamma = 0$ is $\sigma = e_1 = (1, 0, \ldots, 0)^T$. We therefore expect that for $|\gamma|$ small, the optimal value of $\sigma$ in (3.29) will be close to $e_1$, i.e. $\sigma_2, \ldots, \sigma_m$ are expected to be of order $\gamma$. The values $A_{ij}$ with $i, j \geq 2$ therefore come into the value of $f(\sigma)$ only in the third order in $\gamma$ and may be neglected. Then (3.30) becomes 
\[ \sigma_j (\lambda_j + \nu) = -\gamma \sigma_j A_{1j}. \]

Finally, (3.31) shows that $\nu$ is close to $-\lambda_1$. We are then naturally led to choose $\sigma$ according to the equations
\[ \sum_{j=1}^{m} \sigma_j^2 = 1, \quad \sigma_1 \neq 0 \quad \text{and} \quad \frac{\sigma_k}{\sigma_1} = \gamma \cdot \frac{u_1^T X u_k}{\lambda_1 - \lambda_k}, \quad k = 2, \ldots, m. \quad (3.32) \]

Up to the sign of $\sigma$, there is exactly one solution to (3.32), which we plug into (3.29). This leads to
\[ \| M + \gamma X \|_\infty \geq f(\sigma) = \sum_{j=1}^{m} \sigma_j^2 \lambda_j + \gamma \sum_{i,j=1}^{m} \sigma_i \sigma_j A_{ij} \]
\[ = \sigma_1^2 \lambda_1 + \sum_{k=2}^{m} \sigma_k^2 \lambda_k + 2\gamma \sum_{j=2}^{m} \sigma_1 \sigma_j (u_1^T X u_j) + \gamma \sum_{i,j=2}^{m} \sigma_i \sigma_j (u_i^T X u_j) \]
\[ = \sigma_1^2 \lambda_1 + \sum_{k=2}^{m} \sigma_k^2 \lambda_k + 2\gamma \sum_{j=2}^{m} \sigma_1 \sigma_j \frac{(u_1^T X u_k)^2}{(\lambda_1 - \lambda_k)^2} + 2\gamma^2 \sum_{k=2}^{m} \left( \frac{(u_1^T X u_k)^2}{\lambda_1 - \lambda_k} \right)^2 + o(\gamma^2) \quad (3.33) \]
\[ = \sigma_1^2 \lambda_1 + \gamma^2 \sigma_1^2 \sum_{k=2}^{m} \frac{(u_1^T X u_k)^2}{(\lambda_1 - \lambda_k)^2} \left\{ \frac{\lambda_k}{\lambda_1 - \lambda_k} + 2 \right\} + o(\gamma^2) \]
\[ = \sigma_1^2 \left\{ \lambda_1 + \gamma^2 \sum_{k=2}^{m} \frac{(u_1^T X u_k)^2}{(\lambda_1 - \lambda_k)^2} (2\lambda_1 - \lambda_k) \right\} + o(\gamma^2). \]

Furthermore, from $\|\sigma\|_2^2 = 1$, we derive
\[ \sigma_1^2 + \sum_{k=2}^{m} \gamma^2 \sigma_1^2 \frac{(u_1^T X u_k)^2}{(\lambda_1 - \lambda_k)^2} = \sigma_1^2 \left( 1 + \gamma^2 \sum_{k=2}^{m} \frac{(u_1^T X u_k)^2}{(\lambda_1 - \lambda_k)^2} \right) = 1, \]

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which, by the Taylor theorem, leads to
\[
\sigma_1^2 = \left(1 + \gamma^2 \sum_{k=2}^{m} \frac{(u_k^T X u_k)^2}{(\lambda_1 - \lambda_k)^2}\right)^{-1} = 1 - \gamma^2 \sum_{k=2}^{m} \frac{(u_k^T X u_k)^2}{(\lambda_1 - \lambda_k)^2} + o(\gamma^2).
\]

We plug this estimate into (3.33) and get
\[
f(\sigma) = \left(1 - \gamma^2 \sum_{k=2}^{m} \frac{(u_k^T X u_k)^2}{(\lambda_1 - \lambda_k)^2}\right) \cdot \left\{ \lambda_1 + \gamma^2 \sum_{k=2}^{m} \frac{(u_k^T X u_k)^2}{(\lambda_1 - \lambda_k)^2}(2\lambda_1 - \lambda_k) \right\} + o(\gamma^2)
\]
\[
= \lambda_1 + \gamma^2 \sum_{k=2}^{m} \frac{(u_k^T X u_k)^2}{(\lambda_1 - \lambda_k)^2} \left\{ -\frac{\lambda_1}{(\lambda_1 - \lambda_k)^2} + \frac{2\lambda_1 - \lambda_k}{(\lambda_1 - \lambda_k)^2} \right\} + o(\gamma^2)
\]
\[
= \lambda_1 + \gamma^2 \sum_{k=2}^{m} \frac{(u_k^T X u_k)^2}{\lambda_1 - \lambda_k} + o(\gamma^2).
\]

This allows to conclude that
\[
f_X(\gamma) = \frac{\|M + \gamma X\|_\infty}{\sqrt{1 + \gamma^2}} \geq f(\sigma)(1 - \gamma^2/2) = \lambda_1 + \gamma^2 \left( \sum_{k=2}^{m} \frac{(u_k^T X u_k)^2}{\lambda_1 - \lambda_k} - \frac{\lambda_1}{2} \right) + o(\gamma^2).
\]

If \( f_X \) has local maximum at \( \gamma = 0 \), the coefficient at \( \gamma^2 \) has to be smaller or equal to zero, giving (3.22).

\textit{Step 3. Uniqueness of the largest eigenvalue}

We proceed by contradiction. Let (3.25) be fulfilled and let \( M \in \mathcal{A} \) with \( \|M\|_F = 1 \) be a local maximizer of (3.23) with \( \lambda_1 = \lambda_2 = \|M\|_\infty \). The case \( \lambda_1 = \lambda_2 = -\|M\|_\infty \) follows in the same manner. Taking \( X \in \mathcal{S}_X \) with \( X \perp M \) and considering again the function \( f_X \) from (3.16), we can write
\[
f_X(\gamma) = \frac{\|M + \gamma X\|_\infty}{\sqrt{1 + \gamma^2}} \geq \sup_{(\sigma_1, \sigma_2): \sigma_1^2 + \sigma_2^2 = 1} (\sigma_1 u_1 + \sigma_2 u_2)^T (M + \gamma X)(\sigma_1 u_1 + \sigma_2 u_2) + o(\gamma)
\]
\[
= \|M\|_\infty + \gamma \sup_{(\sigma_1, \sigma_2): \sigma_1^2 + \sigma_2^2 = 1} \left\{ \langle \sigma_1^2 u_1^T X u_1 + \sigma_2^2 u_2^T X u_2 + 2\sigma_1 \sigma_2 u_1^T X u_2, \sigma_1 \sigma_2 \rangle \right\} + o(\gamma)
\]

If \( f_X \) has a local maximum at \( \gamma = 0 \), we choose \((\sigma_1, \sigma_2)\) equal to \((1,0), (0,1), \) or \((1,1)/\sqrt{2}\), respectively. We conclude that
\[
u_1^T X u_1 = u_2^T X u_2 = u_1^T X u_2 = 0.
\]

If \( X \in \mathcal{A} \) is not orthogonal to \( M \), we apply (3.34) to \( \frac{X - (X M) M}{\|X - (X M) M\|_2} \), cf. Remark 5, and obtain
\[
u_1^T X u_1 = \langle X, M \rangle \cdot \|M\|_\infty = u_2^T X u_2,
\]
\[
u_1^T X u_2 = 0.
\]

We set \( X_j = P_\mathcal{A}(a_j \otimes a_j) \) and \( E_j = X_j - a_j \otimes a_j \). Then \( X_j \in \mathcal{A} \) and we derive from these conditions
\[
\langle u_1, a_j \rangle^2 + u_1^T E_j u_1 = \langle u_2, a_j \rangle^2 + u_2^T E_j u_2, \quad j = 1, \ldots, m,
\]
\[
\langle u_1, a_j \rangle \cdot \langle u_2, a_j \rangle = -u_1^T E_j u_2, \quad j = 1, \ldots, m.
\]
Solving these equations for $\langle u_1, a_j \rangle^2$, we arrive at

$$\langle u_1, a_j \rangle^2 \leq \frac{|u_2^T \mathcal{E}_j u_2 - u_1^T \mathcal{E}_j u_1| + \sqrt{|u_2^T \mathcal{E}_j u_2 - u_1^T \mathcal{E}_j u_1|^2 + 4(u_1^T \mathcal{E}_j u_2)^2}}{2}$$

$$\leq \frac{2|u_2^T \mathcal{E}_j u_2 - u_1^T \mathcal{E}_j u_1| + 2|u_1^T \mathcal{E}_j u_2|}{2}$$

$$= |u_2^T \mathcal{E}_j u_2 - u_1^T \mathcal{E}_j u_1| + |u_1^T \mathcal{E}_j u_2| \leq 3\|\mathcal{E}_j\|_{\infty}.$$  \hspace{1cm} (3.35)

By assumption $S(a_1, \ldots, a_m) \leq \varepsilon$, Lemma 6.3, and (3.35), we then obtain

$$(1 - \varepsilon)^2 = (1 - \varepsilon)^2 \|u_1\|^2_2 \leq \|A^T u_1\|^2_2 = \sum_{j=1}^{m} \langle u_1, a_j \rangle^2 \leq 3 \sum_{j=1}^{m} \|\mathcal{E}_j\|_{\infty}$$

$$\leq 3 \sum_{j=1}^{m} \|(P_{\tilde{A}} - P_A)(a_j \otimes a_j)\|_F \leq 3m\|P_{\tilde{A}} - P_A\|_{F \rightarrow F},$$

which leads to a contradiction. This finishes the proof of Theorem 3.4.

\[\square\]

### 3.3 Whitening of matrices and \(\varepsilon\)-near-orthonormalization of bases

As we clarify in this section, if the accuracy of the approximation $\tilde{A} \approx A$ is high enough, then, also for systems of vectors \(\{a_i : i = 1, \ldots, m\}\), which are not \(\varepsilon\)-quasi-orthonormal, there is a constructive way, the whitening process we describe below, to render them \(\varepsilon\)-quasi-orthonormal and eventually to distinguish them, as we prove in Section 3.4.

#### 3.3.1 Exact whitening

In this section we explain how we can reduce our analysis to systems \(a_1, \ldots, a_m \in \mathbb{R}^m\) of \(\varepsilon\)-nearly-orthonormal vectors. Assume for the moment \(a_1, \ldots, a_m \in \mathbb{R}^m\) linearly independent unit vectors, but not necessarily orthonormal. We describe below a quite standard orthonormalization procedure, also called in recent literature whitening \([2, 36]\) in the context of symmetric tensor decompositions. It relies on positive definite matrices from the subspace \(\mathcal{A} = \text{span}\{a_i \otimes a_i : i = 1, \ldots, m\}\), which can be easily characterized.

**Lemma 3.5.** Let \(\{a_1, \ldots, a_m\} \subset \mathbb{R}^m\) be arbitrary non-zero vectors in \(\mathbb{R}^m\) and let \(\lambda_1, \ldots, \lambda_m \in \mathbb{R}\) be real numbers. Then the matrix

$$G = \sum_{i=1}^{m} \lambda_i a_i \otimes a_i$$

is positive definite if, and only if, \(\{a_1, \ldots, a_m\}\) are linearly independent and \(\lambda_i > 0\) for all \(i = 1, \ldots, m\).

**Proof.** Let \(\{a_i : i = 1, \ldots, m\}\) be linearly independent and let \(\lambda_i > 0\) for all \(i = 1, \ldots, m\). Let us choose \(x \in \mathbb{R}^m\) with \(x \neq 0\). Then

$$x^TGx = \sum_{i=1}^{m} \lambda_i \langle x, a_i \rangle^2 > 0.$$
If, on the other hand, $G$ is positive definite, and $A \in \mathbb{R}^{m \times m}$ denotes the matrix with columns $a_1, \ldots, a_m$, then

$$0 < x^T G x = x^T A D \lambda A^T x = (A^T x)^T D \lambda (A^T x)$$

for every $x \neq 0$. Here, $D \lambda$ is a diagonal matrix with $\lambda_1, \ldots, \lambda_m$ on the diagonal. As $A^T$ is surjective, $\{a_1, \ldots, a_m\}$ are linearly independent. Furthermore, every non-zero $y \in \mathbb{R}^m$ can be written (in a unique way) as $y = A^T x$ with $x \neq 0$. It follows that $y^T D \lambda y > 0$ for every $y \neq 0$. Therefore, $D \lambda$ is positive definite and $\lambda_i > 0$ for all $i = 1, \ldots, m$.

**Proposition 3.6.** Assume we are given a symmetric and positive definite matrix

$$G = \sum_{i=1}^{m} \lambda_i a_i \otimes a_i, \quad (3.36)$$

and its singular value decomposition

$$G = U D U^T,$$

where $U$ is an orthogonal matrix and $D$ is diagonal matrix with positive diagonal values. If we denote $W = D^{-1/2} U^T$ the so-called whitening matrix, then the system of vectors $\{\sqrt{\lambda_i} W a_i : i = 1, \ldots, m\}$ defines an orthonormal basis and

$$I_m = W G W^T = \sum_{i=1}^{m} \lambda_i W a_i \otimes W a_i$$

is an orthogonal resolution of the identity.

**Proof.** We know that $G \in \mathcal{A}$ can be written as

$$G = U D U^T = \sum_{i=1}^{m} \lambda_i a_i \otimes a_i = AD \lambda A^T, \quad (3.37)$$

where $A \in \mathbb{R}^{m \times m}$ is a matrix with columns $a_1, \ldots, a_m$ and $D \lambda$ is a diagonal matrix with $\lambda_1, \ldots, \lambda_m$ on the diagonal. By Lemma 3.5, $\lambda_i > 0$ for all $i = 1, \ldots, m$. Let $W := D^{-1/2} U^T$. The matrix with columns $\{\sqrt{\lambda_i} W a_i : i = 1, \ldots, m\}$ coincides with $W A D \sqrt{\lambda}$, where $D \sqrt{\lambda}$ is a diagonal matrix with $\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_m}$ on the diagonal. Finally, we observe that

$$(W A D \sqrt{\lambda})(W A D \sqrt{\lambda})^T = W A D \sqrt{\lambda} D \sqrt{\lambda} A^T W^T = W A D \lambda A^T W^T = W G W^T = (D^{-1/2} U^T)(U D U^T)(D^{-1/2} U^T)^T = I_m,$$

hence $W A D \sqrt{\lambda}$ is an orthonormal matrix.

### 3.3.2 Perturbed whitening

Unfortunately in the practice we cannot not access directly of $\mathcal{A} = \text{span}\{a_i \otimes a_i : i = 1, \ldots, m\} \subset \mathbb{R}^{m \times m}$, and therefore it is not possible in general to construct a matrix $G$ as in (3.36). However, the results of Section 3.1 allow us to access an approximating space of symmetric matrices $\hat{\mathcal{A}} \subset \mathbb{R}^{m \times m}$ and in the following we assume that

$$\|P_\mathcal{A} - P_{\hat{\mathcal{A}}}\|_{F \to F} \leq \eta. \quad (3.38)$$

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We assume that we can construct $\tilde{G} \in \tilde{A}$, which is positive definite and define $G = P_A \tilde{G}$. The existence of a positive definite $\tilde{G} \in \tilde{A}$ and algorithmic ways to construct it are discussed in Section 3.3.3 below. We consider their spectral decompositions

$$\tilde{G} = \tilde{U} \tilde{D} \tilde{U}^T \quad \text{and} \quad G = U D U^T.$$ (3.39)

As $G \in A$, it can be again written as in (3.37). Finally, we assume that also $G$ is positive definite, i.e. that $\lambda_i > 0$ for all $i = 1, \ldots, m$. We define again $W := D^{-1/2} U^T$ and its perturbed version $\tilde{W} := \tilde{D}^{-1/2} \tilde{U}^T$. Using this notation together with (3.37) and (3.39), we can quantify the effect of whitening.

**Theorem 3.7.** Let $\gamma, \eta > 0$ be positive real numbers. Let $\|P_A - P_{\tilde{A}}\|_{F \rightarrow F} \leq \eta$ and let $\tilde{G} \in \tilde{A}$ and $G = P_A(\tilde{G})$ be positive definite with $\tilde{G} \succ \gamma I_m$, then

$$S(\sqrt{\lambda_1 \tilde{W} a_1}, \ldots, \sqrt{\lambda_m \tilde{W} a_m}) \leq \frac{\eta \|\tilde{G}\|_F}{\gamma}$$

and \{ $\frac{\tilde{W} a_1}{\|\tilde{W} a_1\|_2}, \ldots, \frac{\tilde{W} a_m}{\|\tilde{W} a_m\|_2}$ \} are $\varepsilon$-nearly-orthonormal, for $\varepsilon = \frac{\sqrt{2\eta \|\tilde{G}\|_F}}{\gamma}$, i.e.,

$$S(\frac{\tilde{W} a_1}{\|\tilde{W} a_1\|_2}, \ldots, \frac{\tilde{W} a_m}{\|\tilde{W} a_m\|_2}) \leq \frac{\sqrt{2\eta \|\tilde{G}\|_F}}{\gamma} =: \varepsilon.$$

**Proof.** We observe that

$$(\tilde{W} A D_{\sqrt{\lambda}}) \cdot (\tilde{W} A D_{\sqrt{\lambda}})^T = \tilde{W} A D_{\lambda} A^T \tilde{W}^T = \tilde{W} G \tilde{W}^T$$

and

$$\tilde{W} G \tilde{W}^T = (\tilde{D}^{-1/2} \tilde{U}^T) \tilde{U} \tilde{D} \tilde{U}^T (\tilde{D}^{-1/2} \tilde{U}^T)^T = I_m.$$ Hence

$$\|(\tilde{W} A D_{\sqrt{\lambda}}) \cdot (\tilde{W} A D_{\sqrt{\lambda}})^T - I_m\|_F = \|\tilde{W} G \tilde{W}^T - \tilde{W} G \tilde{W}^T\|_F = \|\tilde{W} (G - \tilde{G}) \tilde{W}^T\|_F = \|\tilde{D}^{-1/2} \tilde{U}^T (G - \tilde{G}) \tilde{U} \tilde{D}^{-1/2}\|_F \leq \|\tilde{D}^{-1}\| \cdot \|G - \tilde{G}\|_F,$$

which, by Theorem 6.2 in the Appendix, gives the same estimate also for $S(\sqrt{\lambda_1 \tilde{W} a_1}, \ldots, \sqrt{\lambda_m \tilde{W} a_m})$. The second assertion then follows simply by Lemma 6.4.

In Figure 1 we illustrate the result of exact and perturbed whitening of a system of $m = 20$ non-orthogonal vectors.

### 3.3.3 Finding positive definite matrices

In view of Theorem 3.7, we are interested in the following optimization problem. Given an $m$-dimensional subspace $\tilde{A} \subset \mathbb{R}^{m \times m}$ of $m \times m$ symmetric matrices, we would like to answer two questions:

(i) Does $\tilde{A}$ contain a strictly positive matrix?

(ii) And, if this is the case, which positive definite matrix in $\tilde{A}$ achieves the smallest ratio between its Frobenius norm and its smallest eigenvalue?
Figure 1: Density plots of Gramian matrices of the non-orthonormal system \( \{a_i : i = 1, \ldots, m = \} \) for \( m = 20 \) (top left), its exact whitening \( \{\sqrt{\lambda_i} W a_i : i = 1, \ldots, m \} \) (top right) and different perturbed whitenings \( \{\sqrt{\lambda_i} \tilde{W} a_i : i = 1, \ldots, m \} \) for different distortion parameters \( \eta \in \{0.1, 0.01, 0.001, 0.0001\} \). We can observe the increased level of orthonormality for smaller distortion parameters \( \eta \).

Both these tasks can be solved by the following max-min problem

\[
\max_{\tilde{A} \in \tilde{A}} \min_{x \in \mathbb{R}^m, \|x\|_2 = 1} x^T \tilde{A} x.
\] (3.40)

Indeed, the maximizer of (3.40) is the matrix from \( \tilde{A} \), which has the largest minimal eigenvalue among the matrices in \( \tilde{A} \), which have unit Frobenius norm. Furthermore, if the value of (3.40) is zero or negative, there are no positive definite matrices in \( \tilde{A} \).

**Theorem 3.8.** Let \( \tilde{A} \subset \mathbb{R}^{m \times m} \) be a subspace of \( m \times m \) symmetric matrices. Let

\[
\ell(\tilde{A}) := \min_{x \in \mathbb{R}^m, \|x\|_2 = 1} x^T \tilde{A} x
\]
denote the minimal eigenvalue of \( \tilde{A} \in \tilde{A} \). Then \( \tilde{A} \to -\ell(\tilde{A}) \) is a convex function. Furthermore, the solution of the convex minimization problem

\[
\alpha := \min_{\tilde{A} \in \tilde{A}, \|\tilde{A}\|_F \leq 1} (-\ell(\tilde{A}))
\] (3.41)
satisfies $\alpha \leq 0$ with $\alpha = 0$ if, and only if, $\hat{A}$ does not contain any strictly positive definite matrix. If $\alpha < 0$, then the minimizer $A_0$ of (3.41) lies on the sphere $\{A \in \mathcal{A} : \|A\|_F = 1\}$ and coincides with the solution of (3.40).

**Proof.** If $x \in \mathbb{R}^m$ with $\|x\|_2 = 1$ is fixed, then

$$x^T \left( \frac{\hat{A} + \hat{B}}{2} \right) x = \frac{x^T \hat{A} x + x^T \hat{B} x}{2} \geq \frac{\ell(\hat{A}) + \ell(\hat{B})}{2}.$$ 

Taking the infimum over $\|x\|_2 = 1$, we get $\ell(\hat{A})/2 + \ell(\hat{B})/2 \geq \ell(\hat{A})/2 + \ell(\hat{B})/2$. This implies that the function $A \rightarrow \ell(\hat{A})$ is concave. Hence $-\ell$ is convex. As $(-\ell)(0) = 0$, we have $\alpha \leq 0$.

If $\alpha = 0$, then $(-\ell)(\hat{A}) \geq 0$ or, equivalently, $\ell(\hat{A}) \leq 0$ for every $A \in \mathcal{A}$ and $\hat{A}$ does not contain any strictly positive definite matrix.

If $\alpha < 0$, then the minimizer of (3.41) lies on the boundary of the optimization domain due to $\ell(t\hat{A}) = t\ell(\hat{A})$ for every $t > 0$. Hence, in this case,

$$\max_{\hat{A} \in \mathcal{A}} \min_{x \in \mathbb{R}^m, \|x\|_2 = 1} x^T A x = \max_{\hat{A} \in \mathcal{A}, \|\hat{A}\|_F = 1} \ell(\hat{A}) = -\min_{\hat{A} \in \mathcal{A}} (-\ell)(\hat{A}) = -\min_{\hat{A} \in \mathcal{A}, \|\hat{A}\|_F \leq 1} (-\ell)(\hat{A}) = -\alpha.$$ 

\[\square\]

**Remark 6.** Theorem 3.8 translates (3.40) into a convex optimization problem (3.41), cf. [6, 7]. It can be solved in two steps. First, we want to decide if $\hat{A}$ contains a strictly positive matrix. If $\{\hat{A}_1, \ldots, \hat{A}_m\} \subset \mathcal{A}$ is any orthonormal basis of $\hat{A}$, we would like to know if there is a $\xi = (\xi_1, \ldots, \xi_m) \in \mathbb{R}^m$, such that

$$\hat{A} = \xi_1 \hat{A}_1 + \cdots + \xi_m \hat{A}_m > 0.$$ \hspace{1cm} (3.42)

This question is known as feasibility problem of the **linear matrix inequality** (3.42) and we refer to [7, Section 11.4] for a detailed discussion of its solution by interior-point methods. If (3.42) turns out to be feasible, then we can use (for example) an iterative projected subgradient method very much in the spirit of Section 3.5 below to find the solution of (3.40).

**Algorithm 3.2.**

- Fix $\eta > 0$ and let $f^{(0)}(x) = \sum_{i=1}^m g_i^{(0)}(a_i^{(0)} \cdot x)$.
- Compute $\tilde{A}^{(k+1)}$ by using Algorithm 3.1 with accuracy $\eta > 0$ from point values of $f^{(k)}$.
- Define $\tilde{W}^{(k+1)}$ as the whitening matrix of the vectors $\{a_i^{(k)} : i = 1, \ldots, m\}$ by using $\tilde{A}^{(k+1)}$ and algorithm (3.40).
- Define $a_i^{(k+1)} = \tilde{W}^{(k+1)} a_i^{(k)}/\|\tilde{W}^{(k+1)} a_i^{(k)}\|_2$, $i = 1, \ldots, m$.
- Compute $S(a_1^{(k+1)}, \ldots, a_m^{(k+1)})$.
- Denote $f^{(k+1)}(x) = \sum_{i=1}^m g_i^{(k+1)}(a_i^{(k+1)} \cdot x) = f^{(k)}((\tilde{W}^{(k+1)})^T x)$ as in (3.43).
3.3.4 Bootstrap whitening

In view of the simple reformulation
\[
\tilde{f}(\tilde{W}^T x) = \sum_{i=1}^{m} \tilde{g}_i(a_i \cdot \tilde{W}^T x) = \sum_{i=1}^{m} \tilde{g}_i(\sqrt{\lambda_i} \tilde{W} a_i \cdot x) = \tilde{f}(x),
\]
(3.43)

for \( \tilde{g}_i(t) = g_i(t/\sqrt{\lambda_i}) \) and Theorem 3.7, we can further assume without loss of generality that the vectors \( \{a_i : i = 1, \ldots, m\} \) are \( \varepsilon \)-nearly-orthonormal in first place. However, later we will need that \( \varepsilon \) is indeed quite small (certainly smaller than 1 to ensure that our theoretical error estimates are meaningful). In view of Theorem 3.7, this requires \( \eta > 0 \) in the approximation (3.38) also rather small and the identification of a reasonably well-conditioned matrix \( \tilde{G} \).

In this section we report surprising numerical results, obtained by iterating the whitening procedure (Algorithm 3.2). So far, we have not been able to explain this phenomenon analytically, but it is consistently verified in all numerical experiments. It is related to the increasing possibility over the iterations of finding a well-conditioned matrix \( \tilde{G} \) for whitening.

By applying whitening, we can assume through (3.43) that the new function
\[
\tilde{f}(x) = \sum_{i=1}^{m} \tilde{g}_i(\sqrt{\lambda_i} \tilde{W} a_i \cdot x)
\]
has ridge directions \( \sqrt{\lambda_i} \tilde{W} a_i \) which are “more orthogonal” than the original ones \( a_i \) of \( f(x) = \sum_{i=1}^{m} g_i(a_i \cdot x) \). Still, when the distortion parameter \( \eta > 0 \) is not very small (e.g., \( \eta = 0.1 \) for \( m = 20 \)), the level of gained \( \varepsilon \)-near-orthonormality will become rather mild (as also demonstrated in the Figures 1). However, if we apply again the whitening on the previously whitened vectors \( \sqrt{\lambda_i} \tilde{W} a_i \) (for fixed accuracy \( \eta > 0 \)), we surprisingly gain further improved \( \varepsilon \)-near-orthonormality! We implement this bootstrap procedure in Algorithm 3.2 and we show in Figure 2 and Figure 3 corresponding numerical results.

Remark 7. While high accuracy of the approximation \( \tilde{A} \approx A \) is crucial, as we just pointed out, it is important to stress that in our following analysis the \( \varepsilon \)-near-orthonormality is merely useful and technical in order to derive in a relatively simple way theoretical error bounds on the identification of the \( a_i \)’s, see Theorem 3.12 and Theorem 3.16 below. These bounds give interesting guarantees, but their precise form is perhaps of little practical importance, as in cases of vectors \( a_i \)’s which are well-separated (perhaps after just a rough whitening) but not yet \( \varepsilon \)-near-orthonormal for \( \varepsilon \) small, the bounds are either void or vastly overestimate the actual error committed by the reconstruction algorithms, Algorithm 3.3 or Algorithm 3.4. So, the moral is that, as soon as the accuracy \( \tilde{A} \approx A \) is good enough, even just a rough whitening is more than sufficient for our recovery algorithms Algorithm 3.3 or Algorithm 3.4 to recover well the \( a_i \)’s. We extensively illustrate this practical efficiency and robustness in the numerical experiments of Section 5.

3.4 Approximation of weights

We show how to use Theorem 3.4 to develop approximation schemes for sums of ridge functions. We proceed in two steps. In the first step we identify vectors \( \hat{a}_1, \ldots, \hat{a}_m \in \mathbb{R}^m \),
Figure 2: Density plots of Gramian matrices of the non-orthonormal system \( \{ a_i^{(k)} : i = 1, \ldots, m \} \) for \( m = 20 \) for different iterations \( k = 1, \ldots, 6 \) of Algorithm 3.2 for fixed \( \eta = 0.1 \). We observe the increased level of orthonormality of the system along the iterations of Algorithm 3.2.

Figure 3: The values of \( S(a_1^{(k)}, \ldots, a_m^{(k)}) \) for \( m = 20 \) for different iterations \( k = 1, \ldots, 6 \) of Algorithm 3.2 for fixed \( \eta = 0.1 \). We observe the improved level of \( \varepsilon \)-near-orthonormality of the system along the iterations of Algorithm 3.2. Starting with \( S(a_1^{(0)}, \ldots, a_m^{(0)}) \geq S(a_1^{(1)}, \ldots, a_m^{(1)}) > 1 \), one finally obtains \( S(a_1^{(6)}, \ldots, a_m^{(6)}) < 1 \) after \( k = 6 \) iterations.
which approximate the true ridge profiles $a_1,\ldots,a_m$. In the second step we define with their help a function $\hat{f}$, which is the uniform approximation of $f$.

We show, how to use the conditions (3.27) and (3.28) to analyze the minimization problem (3.23). First, we summarize the notation and assumptions used throughout this section. We assume that

- $a_1,\ldots,a_m \in \mathbb{R}^m$ are the unknown weights/ridge profiles,
- $\mathcal{A} = \text{span}\{a_j \otimes a_j, j = 1,\ldots,m\} \subset \mathbb{R}^{m \times m}$,
- the vectors $a_1,\ldots,a_m$ are $\varepsilon$-nearly-orthonormal, i.e., there is an orthonormal basis $w_1,\ldots,w_m$, such that $\left(\sum_{j=1}^m ||a_j - w_j||_2^2\right)^{1/2} = \varepsilon > 0$,
- $\tilde{\mathcal{A}} = \text{span}\{w_j \otimes w_j, j = 1,\ldots,m\}$,
- $\hat{\mathcal{A}}$ is the approximation of $\mathcal{A}$ available after the first step with $\|P_\mathcal{A} - P_{\hat{\mathcal{A}}}\|_{F \rightarrow F} \leq \eta$ (Algorithm 3.1 and Theorem 3.2),
- by Lemma 6.5 in the Appendix we then have $\|P_\mathcal{A} - P_{\hat{\mathcal{A}}}\|_{F \rightarrow F} \leq \|P_\mathcal{A} - P_{\tilde{\mathcal{A}}}\|_{F \rightarrow F} + \|P_{\tilde{\mathcal{A}}} - P_{\hat{\mathcal{A}}}\|_{F \rightarrow F} \leq 4\varepsilon + \eta =: \nu$.

We start with several lemmas needed later on. We will use throughout the notation just introduced.

**Lemma 3.9.** Let $Z \in \hat{\mathcal{A}}$ and $\nu < 1$. Then

$$\|P_{\hat{\mathcal{A}}}(Z)\|_F \leq \|Z\|_F \leq \frac{1}{1 - \nu} \cdot \|P_{\hat{\mathcal{A}}}(Z)\|_F.$$  

In particular, $P_{\hat{\mathcal{A}}}$ is bijective as a map from $\hat{\mathcal{A}}$ to $\tilde{\mathcal{A}}$.

**Proof.** Let $Z \in \hat{\mathcal{A}}$. Then $\|P_{\hat{\mathcal{A}}}Z\|_F \leq \|Z\|_F$ and

$$\|P_{\hat{\mathcal{A}}}Z\|_F \geq \|P_{\tilde{\mathcal{A}}}(Z)\|_F - \|P_{\hat{\mathcal{A}}} - P_{\tilde{\mathcal{A}}}(Z)\|_F \geq \|Z\|_F - \nu \|Z\|_F = (1 - \nu) \|Z\|_F.$$  

The inequality implies the injectivity of $P_{\hat{\mathcal{A}}}$ on $\hat{\mathcal{A}}$ and from Theorem 3.2 we know that $\text{dim}(\tilde{\mathcal{A}}) = \text{dim}(\mathcal{A}) = m$, hence $P_{\hat{\mathcal{A}}}$ is also surjective. \qed

Lemma 3.9 ensures that for any $M \in \tilde{\mathcal{A}}$ with $\|M\|_F = 1$ there exists $Z = \sum_k \sigma_k w_k \otimes w_k \in \hat{\mathcal{A}}$ such that $M = P_{\hat{\mathcal{A}}}(Z)$ and

$$1 \leq \left\| \sum_{k=1}^m \sigma_k w_k \otimes w_k \right\|_F = \|\sigma\|_2 \leq \frac{1}{1 - \nu}. \tag{3.44}$$

We will use this property repetitively below, especially for $M$ being a local maximizer of (3.15).

If $X = w_j \otimes w_j$ and $\|w_j\|_2 = \|u\|_2 = 1$, then

$$\|Xu\|_2^2 = \|\langle w_j, u \rangle w_j\|_2^2 = \|w_j, u\|_2^2 = (w_j^T w_j)(w_j^T u) = u^T X u.$$  

If $X = P_{\hat{\mathcal{A}}}(w_j \otimes w_j)$ instead, we expect the difference between $\|Xu\|_2^2$ and $u^T X u$ to be small. This statement is made precise in the following lemma.
Lemma 3.10. Let \( W_j = w_j \otimes w_j, X = P_\hat{A}(W_j) \) and \( \|u\|_2 = 1 \). Then

\[
\|Xu\|^2 - u^TXu \leq 2\nu.
\]

Proof. Indeed, using \( W_j = P_\hat{A}(W_j) = W_j^2 \) we obtain

\[
|Xu|^2 - u^TXu = |\langle P_\hat{A}(W_j)u, P_\hat{A}(W_j)u \rangle - u^T(P_\hat{A}W_j)u|
\]

\[
\leq \|P_\hat{A}(W_j) - P_\hat{A}\|_\infty \leq \|P_\hat{A}(W_j) - P_\hat{A}\|_\infty
\]

\[
\leq \|P_\hat{A}(W_j) - P_\hat{A}(W_j)\|_\infty + \|P_\hat{A}(W_j) - P_\hat{A}(W_j)\|_\infty
\]

\[
\leq \|P_\hat{A}(W_j) - P_\hat{A}(W_j)\|_\infty + \|P_\hat{A}(W_j) - P_\hat{A}(W_j)\|_\infty
\]

\[
\leq \|P_\hat{A}(W_j) - P_\hat{A}(W_j)\|_\infty + \|P_\hat{A}(W_j) - P_\hat{A}(W_j)\|_\infty \leq 2\nu. \quad \Box
\]

We show that the local maximizers \( M \) of (3.15) are (possibly after replacing \( M \) by \( -M \)) nearly positive semi-definite.

Lemma 3.11. Let \( \nu \leq 1/4 \) and let \( M \) be a local maximizer of (3.23) with \( \|M\|_\infty = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m \) being its eigenvalues. Then

\[
\lambda_m \geq -\frac{2\nu}{\lambda_1^2} - 4\nu. \quad (3.45)
\]

Proof. We plug \( X = P_\hat{A}(w_j \otimes w_j) \) into (3.27) and obtain

\[
u^T P_\hat{A}(w_j \otimes w_j) u_1 = \langle P_\hat{A}(w_j \otimes w_j), M \rangle \lambda_1.
\]

We observe now that from \( \|P_\hat{A} - P_\hat{A}\|_F \leq \nu \), we have \( \|u_1^T(P_\hat{A} - P_\hat{A})(w_j \otimes w_j)u_1\| \leq \nu \), implying \( u_1^T(P_\hat{A} - P_\hat{A})(w_j \otimes w_j)u_1 \geq -\nu \) and

\[
-\nu \leq (w_j, u_1)^2 + u_1^T(P_\hat{A} - P_\hat{A})(w_j \otimes w_j)u_1 = u_1^T(w_j \otimes w_j)u_1 + u_1^T(P_\hat{A} - P_\hat{A})(w_j \otimes w_j)u_1
\]

\[
u \leq w_j, u_1 \rangle + \sum_{k=1}^m \sigma_k \langle P_\hat{A}(w_j \otimes w_j), P_\hat{A}(w_k \otimes w_k) \rangle
\]

Below we often use for \( Z \in \hat{A} \) that \( \|P_\hat{A}Z\|_F = \|P_\hat{A}Z\|_F = \|P_\hat{A}Z + (P_\hat{A} - P_\hat{A})Z\|_F \geq (1 - \nu)\|Z\|_F \). If \( \sigma_j < 0 \) for any \( j \), we use Lemma 3.9, (3.44), and the relationship \( \langle P_\hat{A}(w_j \otimes w_j), (w_k \otimes w_k) \rangle = \delta_{jk} \) to derive the estimates

\[
-\nu/\lambda_1 \leq \nu \langle P_\hat{A}(w_j \otimes w_j), P_\hat{A}(w_k \otimes w_k) \rangle
\]

\[
\leq \sigma_j (1 - \nu)^2 \left( \sum_{k \neq j} \sigma_k \langle P_\hat{A}(w_j \otimes w_j), P_\hat{A}(w_k \otimes w_k) \rangle \right)^{1/2}
\]

\[
\leq \sigma_j (1 - \nu)^2 + \|P_\hat{A} - P_\hat{A}\|_F \leq \sigma_j (1 - \nu)^2 + \frac{\nu}{1 - \nu}
\]

We conclude that

\[
\min_{j=1, \ldots, m} \sigma_j \geq \frac{2\nu}{\lambda_1^2} + \frac{\nu}{(1 - \nu)^2}
\]
Finally,

\[
\lambda_m = u_m^T M u_m = \sum_{j=1}^m \sigma_j \langle P_{\tilde{A}}(w_j \otimes w_j), u_m \otimes u_m \rangle
\]

\[
= \sum_{j=1}^m \sigma_j \langle w_j \otimes w_j, u_m \otimes u_m \rangle + \sum_{j=1}^m \sigma_j \langle (P_{\tilde{A}} - P_A)(w_j \otimes w_j), u_m \otimes u_m \rangle
\]

\[
\geq (\min_j \sigma_j) \sum_{j=1}^m (w_j, u_m)^2 + \left( \langle (P_{\tilde{A}} - P_A)(\sum_{j=1}^m \sigma_j w_j \otimes w_j), u_m \otimes u_m \rangle \right)
\]

\[
\geq (\min_j \sigma_j) - \|P_{\tilde{A}} - P_A\| \cdot \left\| \sum_{j=1}^m \sigma_j w_j \otimes w_j \right\|_F
\]

\[
\geq (\min_j \sigma_j) - \frac{\nu}{1 - \nu} \geq - \left( \frac{\nu}{\lambda_1}, \frac{\nu}{1 - \nu} \right) \cdot \frac{1}{(1 - \nu)^2} - \frac{\nu}{1 - \nu},
\]

where in the second last inequality we used (3.44), and the result follows now by simple algebraic computations for \(\nu \leq 1/4\). \(\square\)

The recovery algorithm based on the optimization problem (3.23) is quite straightforward. We show that the eigenvector corresponding to the largest eigenvalue of any of its local maximizers is actually close to one of the ridge profiles.

**Algorithm 3.3.**

- Let \(M\) be a local maximizer of (3.23).
- If \(\|M\|_\infty\) is not an eigenvalue of \(M\), replace \(M\) by \(-M\).
- Denote by \(\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m\) the eigenvalues of \(M\) arranged in decreasing order.
- Take the eigenvalue decomposition of \(M\), i.e. \(M = \sum_{j=1}^m \lambda_j u_j \otimes u_j\).
- Put \(\hat{a} := u_1\).

The performance of Algorithm 3.3 is guaranteed by the following theorem.

**Theorem 3.12.** If \(0 < \nu < 1/(cm)\), for a suitable constant \(c > 6\), then there is \(j_0 \in \{1, \ldots, m\}\), such that the vector \(\hat{a}\) found by Algorithm 3.3 satisfies \(\|\hat{a} - a_{j_0}\|_2 \leq 5\nu\).

The proof of this theorem, which we report below, is fundamentally based on proving the following bound

\[
\|M\|_\infty = \lambda_1 \geq 1 - c'\nu,
\]

(3.46)

for some \(c' > 0\) and for any local maximizers \(M\) of (3.23). This will allow to ensure a sufficient spectral gap to apply the Wedin’s bound (Theorem 6.6) for showing good approximation properties of \(\hat{a}\) as in Algorithm 3.3 to one of the ridge directions \(a_1, \ldots, a_m\). We shall obtain (3.46) by a bootstrap argument: first we need to establish a weaker bound

\[
\lambda_1 > \frac{\nu}{1 - \nu},
\]

and use it for deducing (3.46).
Lemma 3.13. Assume $0 < \nu < 1/(6m)$. Then the following inequalities hold:

$$\|Xu_1\|_2^2 \leq \lambda_1^2 \cdot \frac{1 + \langle X, M \rangle^2}{2} + 3\nu,$$

(3.47)

for any $X \in \tilde{A}$ such that $\|X\|_F \leq 1$ and

$$\lambda_1 > \frac{\nu}{1 - \nu}.$$  \hspace{1cm} (3.48)

Proof. Let $M$ be any of the local maximizers of (3.23) with $\lambda_1 = \|M\|_\infty$. Further let $X \in \tilde{A}$. We estimate the left-hand side of (3.28) using (3.27)

$$2 \sum_{k=2}^m (u_k^T Xu_k)^2 \geq 2 \min \left( \frac{1}{\lambda_1 - \lambda_k} \right) \sum_{k=2}^m (u_k^T Xu_k)^2 = \frac{2}{\lambda_1 - \lambda_m} \sum_{k=2}^m \langle Xu_1, u_k \rangle^2$$

$$= \frac{2}{\lambda_1 - \lambda_m} \left( \|Xu_1\|_2^2 - \langle Xu_1, u_1 \rangle^2 \right)$$

$$= \frac{2}{\lambda_1 - \lambda_m} \left( \|Xu_1\|_2^2 - \lambda_1^2 \langle X, M \rangle^2 \right).$$

Together with (3.28), this leads to

$$\frac{2}{\lambda_1 - \lambda_m} \left( \|Xu_1\|_2^2 - \lambda_1^2 \langle X, M \rangle^2 \right) \leq \lambda_1 (\|X\|_F^2 - \langle X, M \rangle^2).$$

If moreover $\|X\|_F \leq 1$, $\nu \leq \frac{1}{4}$, and using (3.45) we conclude that

$$\|Xu_1\|_2^2 \leq \frac{\lambda_1 (\lambda_1 - \lambda_m)}{2} (\|X\|_F^2 - \langle X, M \rangle^2) + \lambda_1^2 \langle X, M \rangle^2$$

$$\leq \frac{\lambda_1 (\lambda_1 - \lambda_m)}{2} + \lambda_1 \left( \lambda_1 + \frac{\lambda_1 - \nu}{\lambda_1} \right) \cdot \frac{1 - \langle X, M \rangle^2}{2}$$

$$\leq \frac{\lambda_1^2}{2} \cdot \frac{1 + \langle X, M \rangle^2}{2} + 2\lambda_1 \left( \frac{\nu}{\lambda_1} + 2\nu \right) \cdot \frac{1 - \langle X, M \rangle^2}{2}$$

$$\leq \frac{\lambda_1^2}{2} \cdot \frac{1 + \langle X, M \rangle^2}{2} + 3\nu.$$  \hspace{1cm} (3.49)

Let us choose $X = \sum_{k=1}^m x_k P_{\tilde{A}}(w_k \otimes w_k)$ with $\|x\|_2 \leq 1$, a generic element in $\tilde{A}$ such that $\|X\|_F \leq 1$. We compute

$$\|Xu_1\|_2 = \left\| \sum_{k=1}^m x_k P_{\tilde{A}}(w_k \otimes w_k)u_1 \right\|_2$$

$$\geq \left\| \sum_{k=1}^m x_k (w_k \otimes w_k)u_1 \right\|_2 - \left\| \sum_{k=1}^m x_k (P_{\tilde{A}} - P_{\tilde{A}})(w_k \otimes w_k)u_1 \right\|_2$$

$$\geq (1 - \nu) \left\| \sum_{k=1}^m x_k (u_1, w_k)w_k \right\|_2 = (1 - \nu) \left( \sum_{k=1}^m x_k^2 (u_1, w_k)^2 \right)^{1/2}. $$

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By choosing $x_k = 1/\sqrt{m}$ for all $k = 1, \ldots, m$, we obtain
\[
\|X u_1\|_2^2 \geq \frac{(1 - \nu)^2}{m} \sum_{k=1}^{m} (u_1, w_k)^2 = \frac{(1 - \nu)^2}{m}.
\]

Combining with (3.49) yields
\[
\frac{(1 - \nu)^2}{m} \leq \|X u_1\|_2^2 \leq \lambda_1^2 \cdot \frac{1 + (X, M)^2}{2} + 3\nu \leq \lambda_1^2 + 3\nu,
\]
or
\[
\lambda_1^2 \geq \frac{(1 - \nu)^2}{m} - 3\nu.
\]

In order to show that $\lambda_1 > \frac{\nu}{1 - \nu}$, it is in fact sufficient to show that for $\nu \leq 1/(6m)$
\[
\frac{(1 - \nu)^2}{m} - 3\nu > \frac{16}{9}\nu^2.
\]

Indeed one would have then
\[
\lambda_1^2 \geq \frac{(1 - \nu)^2}{m} - 3\nu > \frac{\nu^2}{(1 - 1/4)^2} \geq \frac{\nu^2}{(1 - \nu)^2}
\]

The quadratic inequality (3.50) is in fact fulfilled for $0 < \nu < 1/(6m)$.

**Proof of Theorem 3.12.** Let $M$ be any of the local maximizers of (3.23) with $\lambda_1 = \|M\|_\infty$. Further let $X \in \tilde{A}$. If $X = P_{\tilde{A}}(\omega_j \otimes \omega_j)$ by Lemma 3.10
\[
\|X u_1\|_2^2 \geq u_1^T X u_1 - 2\nu = \lambda_1 (X, M)_F - 2\nu.
\]

Using (3.47), we then arrive at
\[
\lambda_1 (X, M)_F - 2\nu \leq \lambda_1^2 \cdot \frac{1 + (X, M)^2}{2} + 3\nu.
\]

This can be further rewritten as
\[
0 \leq \lambda_1^2 - 1 + (1 - \lambda_1 (X, M)_F)^2 + 10\nu.
\]

Assume now that there exists $Z = \sum_{k=1}^{m} \sigma_k (w_k \otimes w_k) \in \hat{A}$ such that $M = P_{\hat{A}} Z$ and using (3.44), we can estimate $\lambda_1$ from above
\[
\lambda_1 = u_1^T M u_1 = u_1^T \left( \sum_{k=1}^{m} \sigma_k P_{\hat{A}}(w_k \otimes w_k) \right) u_1
\]
\[
= u_1^T (P_{\hat{A}} - P_{\tilde{A}}) \left( \sum_{k=1}^{m} \sigma_k (w_k \otimes w_k) \right) u_1 + u_1^T \left( \sum_{k=1}^{m} \sigma_k (w_k \otimes w_k) \right) u_1
\]
\[
\leq \nu \left\| \sum_{k=1}^{m} \sigma_k (w_k \otimes w_k) \right\|_F^2 + \sum_{k=1}^{m} \sigma_k (w_k, u_1)^2 \leq \frac{\nu}{1 - \nu} + \max_{j=1, \ldots, m} \sigma_j.
\]

From Lemma 3.13 and in particular by (3.48) we deduce that
\[
\max_{j=1, \ldots, m} \sigma_j \geq \lambda_1 - \frac{\nu}{1 - \nu} > 0.
\]
Hence there exists certainly some \( j \) for which \( \sigma_j > 0 \). If \( X = P_{\tilde{A}}(w_j \otimes w_j) \) we get for \( \sigma_j > 0 \)

\[
\langle X, M \rangle = \langle P_{\tilde{A}}(w_j \otimes w_j), M \rangle = \langle P_{\tilde{A}}(w_j \otimes w_j), \sum_{k=1}^{m} \sigma_k P_{\tilde{A}}(w_k \otimes w_k) \rangle \\
= \sigma_j \langle P_{\tilde{A}}(w_j \otimes w_j), P_{\tilde{A}}(w_j \otimes w_j) \rangle + \langle w_j \otimes w_j, \sum_{k \neq j} \sigma_k (P_{\tilde{A}} - P_{\tilde{A}})(w_k \otimes w_k) \rangle \\
= \sigma_j \langle P_{\tilde{A}}(w_j \otimes w_j), w_j \otimes w_j \rangle + \langle (P_{\tilde{A}} - P_{\tilde{A}}) \left( \sum_{k \neq j} \sigma_k w_j \otimes w_j \right), w_k \otimes w_k \rangle \\
\geq \sigma_j \cdot (1 - \nu) - \nu \|\sigma\|_2 \geq \sigma_j \cdot (1 - \nu) - \frac{\nu}{1 - \nu}.
\]

We conclude, that there is \( j_0 \in \{1, \ldots, m\} \) with

\[
\langle P_{\tilde{A}}(w_{j_0} \otimes w_{j_0}), M \rangle \geq (1 - \nu) \max_{j=1,\ldots,m} \sigma_j - \frac{\nu}{1 - \nu}, \tag{3.53}
\]

Combining (3.53) with (3.52), we obtain for \( \nu \leq 1/4 \)

\[
\langle P_{\tilde{A}}(w_{j_0} \otimes w_{j_0}), M \rangle \geq (\lambda_1 - \frac{\nu}{1 - \nu}) \cdot (1 - \nu) - \frac{\nu}{1 - \nu} \\
= \lambda_1 (1 - \nu) - \frac{2 - \nu}{1 - \nu} \geq \lambda_1 (1 - \nu) - \frac{5\nu}{2}
\]

and

\[
0 \leq 1 - \lambda_1 \langle P_{\tilde{A}}(w_{j_0} \otimes w_{j_0}), M \rangle \leq 1 - \lambda_1^2 (1 - \nu) + \frac{5\lambda_1 \nu}{2}. \tag{3.54}
\]

Finally, (3.51) with (3.54) give

\[
0 \leq \lambda_1^2 - 1 + \left( 1 - \lambda_1^2 (1 - \nu) + \frac{5\lambda_1 \nu}{2} \right)^2 + 10\nu \\
= \lambda_1^4 (\lambda_1^2 - 1) + \nu \left\{ -2\lambda_1^4 + \nu \lambda_1^4 - 2\lambda_1^2 + \frac{25}{4} \lambda_1^2 \nu + 5\lambda_1 - 5\lambda_1^3 (1 - \nu) + 10 \right\} \\
\leq \lambda_1^4 (\lambda_1^2 - 1) + \tilde{c} \nu.
\]

By solving the latter quadratic inequality, only two solutions are possible \( \lambda_1 \geq 1 - c' \nu \) and \( \lambda_1 \leq c'' \sqrt{\nu} \), for some \( c', c'' > 0 \). Since \( \lambda_1 \geq 1/\sqrt{m} \) for any \( \nu > 0 \), if \( \nu < 1/(cm) \) for \( c = (c'')^2 \) then the second option \( \lambda_1 \leq c'' \sqrt{\nu} \) must be excluded. As we assume that \( \nu < 1/(cm) \) for a suitable constant \( c > 6 \) large enough, we conclude, that not only \( \lambda_1 > \frac{\nu}{1 - \nu} \), but we indeed have the significantly better lower bound

\[
\lambda_1 \geq 1 - c' \nu,
\]

for some \( c' > 0 \). Finally, we apply the Wedin’s bound, Theorem 6.6 in the Appendix, to

\[
\tilde{B} = M = \sum_{j=1}^{m} |\lambda_j| \text{sgn}\lambda_j u_j \otimes u_j \quad \text{and} \quad B = \sum_{k=1}^{m} |\sigma_k| \text{sgn}\sigma_k w_k \otimes w_k.
\]

We assume without loss of generality that \( \sigma_1 = \max_{k=1,\ldots,m} |\sigma_k| \). We observe that

\[
\|\tilde{B} - B\|_F = \|P_{\tilde{A}}(B) - B\|_F = \|(P_{\tilde{A}} - P_{\tilde{A}})(B)\|_F \leq \nu \|B\|_F = \nu \|\sigma\|_2 \leq \frac{\nu}{1 - \nu}.
\]

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Moreover
\[
\left( \sum_{j=1}^{m} |\lambda_j|^2 \right)^{1/2} \leq 1 \text{ and } \lambda_1 \geq 1 - c' \nu
\]
imply \( |\lambda_k| \leq c' \nu \) for all \( k = 2, \ldots, m \). Moreover, \( \left( \sum_{k=1}^{m} |\sigma_k|^2 \right)^{1/2} \leq \frac{1}{1-\nu} \) and
\[
\frac{1}{1-\nu} \geq \sigma_1 \geq \lambda_1 - \frac{\nu}{1-\nu} \geq 1 - \left( \frac{1}{1-\nu} + c' \right) \nu
\]
imply \( |\sigma_k| \leq \frac{2 + c'(1-\nu)}{1-\nu} \nu \) for all \( k = 2, \ldots, m \). We deduce that we can choose \( \bar{\alpha} \geq \frac{1}{2} \) as in Theorem 6.6 for \( 0 < \nu < \nu_0 \) small enough, i.e.,
\[
\min_k |\lambda_1 - \sigma_k| \geq \left| 1 - c' \nu - \frac{2 + c'(1-\nu)}{1-\nu} \right| \bar{\alpha} \geq 1/2,
\]
and
\[
|\lambda_1| \geq |1 - c' \nu| \geq \bar{\alpha} \geq 1/2,
\]
are verified for \( 0 < \nu < \nu_0 \) small enough. We do not specify \( \nu_0 > 0 \) but its existence follows by a simple continuity argument. We therefore obtain \( \|u_1 \otimes u_1 - w_1 \otimes w_1\|_F \leq 4\nu \). After a possible sign change of \( w_1 \), we can assume that \( \langle u_1, w_1 \rangle \geq 0 \) and obtain
\[
16\nu^2 \geq \|u_1 \otimes u_1 - w_1 \otimes w_1\|_F^2 = 2(1 - \langle u_1, w_1 \rangle^2) \geq 2(1 - \langle u_1, w_1 \rangle) = \|u_1 - w_1\|_2^2
\]
and, finally,
\[
\|u_1 - a_1\|_2 \leq \|u_1 - w_1\|_2 + \|w_1 - a_1\|_2 \leq 4\nu + \varepsilon \leq 5\nu.
\]
\[ \square \]

3.5 A simple iterative algorithm

Let us describe in this section how to approach practically the solution of the nonlinear program (3.1). Let us introduce first for a given parameter \( \gamma > 1 \) an operator acting on the singular values of a matrix \( X = U \Sigma V^T \) as follows. If \( \Sigma \in \mathbb{R}^{m \times m} \) is a diagonal matrix with the singular values of \( X \) denoted by \( \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m \) on the diagonal, we set
\[
\Pi_\gamma(X) = \frac{1}{\sqrt{\gamma^2 \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_m^2}} U \begin{pmatrix}
\gamma \sigma_1 & 0 & \cdots & 0 \\
0 & \sigma_2 & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots \\
0 & \cdots & 0 & \sigma_m
\end{pmatrix} V^T.
\]

Notice that \( \Pi_\gamma \) maps any matrix \( X \) onto a matrix of unit Frobenius norm, simply exalting the first singular value and damping the others. It is not a linear operator. Furthermore, the definition of \( \Pi_\gamma(X) \) is not well-posed if \( \sigma_1 = \sigma_2 \geq \sigma_3 \geq \cdots \geq \sigma_m \) and in this case it is assumed that a choice of ordering is made for just this one application of \( \Pi_\gamma(\cdot) \). Notice that if \( \sigma_1 > 1/\sqrt{2} \) and \( \|X\|_F \leq 1 \), then \( \sigma_1 > \sigma_2 \) and \( \Pi_\gamma(X) \) is well-defined. This is the case for example under the conditions of Lemma 3.15.

We propose the following algorithm
Algorithm 3.4.

- Fix a suitable parameter $\gamma > 1$.
- Generate an initial guess $X^0 \in \tilde{A}$ and $\|X^0\|_F = 1$ at random.
- For $\ell \geq 0$:
  
  \[
  X^{\ell+1} := P_{\tilde{A}} \Pi_{\gamma}(X^\ell).
  \]

This algorithm performs essentially an iteratively projected subgradient ascent method as the two operations executed within the loop are respectively a subgradient ascent step towards the maximization of the spectral norm by means of $\Pi_{\gamma}$, and a projection back onto $\tilde{A}$ by $P_{\tilde{A}}$.

In the following we analyze some of the convergence properties of this algorithm and its relationship to (3.1). Assume for a moment now that $\tilde{A} = A$ and that $a_1, \ldots, a_m$ are orthonormal. In this case the algorithm can be rather trivially analyzed and performs a straightforward computation of one of the maximizers of (3.1). As we shall see later, such maximizer in this case coincides (up to the sign) with one of the matrices $a_j \otimes a_j$.

\textbf{Proposition 3.14.} Assume that $\tilde{A} = A$ and that $a_1, \ldots, a_m$ are orthonormal. Let $\gamma > \sqrt{2}$ and let $\|X^0\|_\infty > 1/\sqrt{\gamma^2 - 1}$. Then there exists $\mu_0 < 1$ such that

\[
\begin{align*}
1 - \|X^{\ell+1}\|_\infty & \leq \mu_0 \left( 1 - \|X^\ell\|_\infty \right), \quad \text{for all } \ell \geq 0.
\end{align*}
\]  

(3.55)

Being the sequence $(X^\ell)_\ell$ made of matrices with Frobenius norm bounded by 1, we conclude that any accumulation point of it has both unit Frobenius and spectral norm and therefore it has to coincide with one maximizer of (3.1).

\textbf{Proof.} We can assume now that $X^0$ can already be expressed in terms of its singular value decomposition $X^0 = \sum_{j=1}^m \sigma_j(X^0) a_j \otimes a_j$. Since at each iteration $\|X^\ell\|_F \leq 1$ or $1 \geq \sum_{j=1}^m \sigma_j(X^\ell)^2$, it is a straightforward observation that

\[
\|X^{\ell+1}\|_\infty = \sigma_1(X^{\ell+1}) = \frac{\gamma \sigma_1(X^\ell)}{\sqrt{\gamma^2 \sigma_1(X^\ell)^2 + \sigma_2(X^\ell)^2 + \cdots + \sigma_m(X^\ell)^2}}
\]  

(3.56)

\[
\geq \frac{\gamma \sigma_1(X^\ell)}{\sqrt{(\gamma^2 - 1) \sigma_1(X^\ell)^2 + 1}}.
\]

Using elementary calculations we further estimate

\[
1 - \sigma_1(X^{\ell+1}) \leq \frac{\sqrt{(\gamma^2 - 1) \sigma_1(X^\ell)^2 + 1} - \gamma \sigma_1(X^\ell)}{\sqrt{(\gamma^2 - 1) \sigma_1(X^\ell)^2 + 1}}
\]  

(3.57)

\[
= \frac{1 - \sigma_1(X^\ell)^2}{\sqrt{(\gamma^2 - 1) \sigma_1(X^\ell)^2 + 1} + \gamma \sigma_1(X^\ell)} \left( \frac{1 - \sigma_1(X^\ell)^2}{\sqrt{(\gamma^2 - 1) \sigma_1(X^\ell)^2 + 1}} \right) \leq \frac{2(1 - \sigma_1(X^\ell)^2)}{(\gamma^2 - 1) \sigma_1(X^\ell)^2 + 1}
\]

and we get (3.55) with

\[
\mu_0 := \frac{2}{(\gamma^2 - 1) \|X^0\|_\infty^2 + 1} < 1.
\]
Let us now move away from the ideal case of the $\tilde{A} = A$ and assume that $\tilde{A}$ is only a good approximation to $A$, in the sense that $\|P_{\tilde{A}} - P_A\| \leq \varepsilon$.

**Remark 8.** As we learned already in the previous section, we can retain without loss of generality the assumption of $a_1, \ldots, a_m$ being orthonormal to a certain extent. Indeed, were $\{a_1, \ldots, a_m\}$ just $\varepsilon$-near-orthonormal and $\{w_1, \ldots, w_m\}$ its approximating orthonormal basis, then we could denote $\alpha_i = a_i a_i^T \in \mathbb{R}^{m \times m}$, $\omega_i = w_i w_i^T \in \mathbb{R}^{m \times m}$, $A = \text{span}\{a_1, \ldots, a_m\}$ and $\tilde{A} = \text{span}\{\omega_1, \ldots, \omega_m\}$. It is shown in Lemma 6.3 (iv), that $\left(\sum_{i=1}^{m} \|\alpha_i - \omega_i\|_F^2\right)^{1/2} \leq 2\varepsilon$.

Combining this result with Lemma 6.5 we would obtain $\|P_A - P_{\tilde{A}}\|_{F \rightarrow F} \leq 8\varepsilon$. Hence, at the price of changing slightly the reference orthonormal basis and accepting some additional approximation error of order $\varepsilon$, also in the case of a $\varepsilon$-near-orthonormal system of vectors we can reduce the arguments to the case of an orthonormal system.

Unfortunately, in the perturbed case $\tilde{A} \neq A$, there is no direct way of estimating $\|X^{t+1}\|_\infty$ by some function of $\|X^t\|_\infty$ as it is done in (3.56) as the singular value decompositions of the matrices $X^{t+1}$ and $X^t$ are in principle different. However, the singular vectors of both these matrices can be approximated by $\{a_1, \ldots, a_m\}$ (we reiterate that here we assume them orthonormal) and we need to take advantage of this reference orthonormal system. First, we need to show a certain continuity property of the operator $\Pi_{\gamma}$.

**Lemma 3.15.** Assume $X$, $\tilde{X}$ to be two matrices in $\mathbb{R}^{m \times m}$ with respective singular value decompositions $X = U\Sigma V^T$ and $\tilde{X} = \tilde{U}\Sigma \tilde{V}^T$. Let us also assume that $\|X - \tilde{X}\|_F \leq \varepsilon$ for some $0 < \varepsilon < 1$. Assume additionally that $\max\{\|\tilde{X}\|_F, \|X\|_F\} \leq 1$ and $\sigma_1(X) \geq t_0 := \frac{1}{\sqrt{2}} + \varepsilon + \xi$, for $\xi > 0$. Then, for $\gamma > 1$

$$\|\Pi_{\gamma}(X) - \Pi_{\gamma}(\tilde{X})\|_F \leq 2^{3/2}\varepsilon + \frac{4\varepsilon}{\xi} + 2\sqrt{1 - (t_0 - \varepsilon)} := \mu_1(\gamma, t_0, \varepsilon)$$

(3.58)

Notice in particular that $\mu_1(\gamma, t_0, \varepsilon) \rightarrow 0$ for $(t_0, \varepsilon) \rightarrow (1, 0)$.

**Proof.** As $\sigma_1 := \sigma_1(X) \geq t_0$ and $\sigma_1^2 + \cdots + \sigma_m^2 \leq 1$, we have also $\sum_{j=2}^{m} \sigma_j^2 \leq 1 - t_0^2$.

By the assumption $\|X - \tilde{X}\|_F \leq \varepsilon$ and by the well known Mirsky’s bound we have that $\|\Sigma - \tilde{\Sigma}\|_F \leq \varepsilon$.

Hence, $\hat{\sigma}_1 := \sigma_1(\tilde{X}) \geq t_0 - \varepsilon$, $\hat{\sigma}_j := \sigma_j(\tilde{X}) \leq \sqrt{1 - t_0^2} + \varepsilon$ and

$$|\hat{\sigma}_1 - \sigma_j| \geq t_0 - \varepsilon - \sqrt{1 - t_0^2} := \delta > 0,$$

for all $j = 2, \ldots, m$. The positivity of $\hat{\delta} > 0$ comes from the assumption that $t_0 = \frac{1}{\sqrt{2}} + \varepsilon + \xi$. Hence, by applying Wedin’s bound, Theorem 6.6 in Appendix, we easily obtain

$$\max\{\|u_1 u_1^T - \tilde{u}_1 \tilde{u}_1^T\|_F, \|v_1 v_1^T - \tilde{v}_1 \tilde{v}_1^T\|_F\} \leq \frac{2}{t_0 - \varepsilon - \sqrt{1 - t_0^2}} \varepsilon \leq \frac{2\varepsilon}{\xi},$$

(3.59)

The last inequality comes from $1 < 2(t_0 - \varepsilon - \xi)^2 < (t_0 - \varepsilon - \xi)^2 + t_0^2$. For later use we notice already that for any unit-norm vectors $x, \tilde{x} \in \mathbb{R}^m$

$$\|xx^T - \tilde{xx}^T\|_F^2 = \|xx^T\|_F^2 + \|\tilde{xx}^T\|_F^2 - 2\langle xx^T, \tilde{xx}^T\rangle = 2(1 - \langle x, \tilde{x}\rangle^2)$$

and

$$\langle x, \tilde{x}\rangle = \sqrt{1 - \frac{\|xx^T - \tilde{xx}^T\|_F^2}{2}} \geq 1 - \frac{\|xx^T - \tilde{xx}^T\|_F^2}{2}.$$

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If moreover $\langle x, \tilde{x}\rangle \geq 0$, we get
\[
\|x - \tilde{x}\|^2 = 2(1 - \langle x, \tilde{x}\rangle) \leq \|xx^T - \tilde{x}\tilde{x}^T\|^2_F.
\] (3.60)

We now address (3.58) by considering the estimates of different components of the singular value decompositions. We start by comparing the first singular value components. To simplify the notation, we set for $s = (s_1, \ldots, s_m)$
\[
\pi_\gamma(s) = \pi_\gamma(s_1, \ldots, s_m) = \frac{\gamma s_1}{\sqrt{s_1^2 + s_2^2 + \cdots + s_m^2}}.
\]
We first derive a bound for $\|u_1 \pi_\gamma(\sigma)v_1^T - \tilde{u}_1 \pi_\gamma(\tilde{\sigma})\tilde{v}_1^T\|_F$, where $\sigma = (\sigma_1, \ldots, \sigma_m)$ and similarly for $\tilde{\sigma} = (\tilde{\sigma}_1, \ldots, \tilde{\sigma}_m)$.

For that, we need first to show the Lipschitz continuity of the function $s \mapsto \pi_\gamma(s)$. From
\[
|\partial_{s_1} \pi_\gamma(s_1, \ldots, s_m)| = \left| \frac{\gamma (s_2^2 + \cdots + s_m^2)}{(\gamma s_1^2 + s_2^2 + \cdots + s_m^2)^{3/2}} \right|
\]
and
\[
|\partial_{s_j} \pi_\gamma(s_1, \ldots, s_m)| = \left| \frac{\gamma s_1 s_j}{(\gamma s_1^2 + s_2^2 + \cdots + s_m^2)^{3/2}} \right|
\]
we obtain for $1 \leq s_1 > t_0 - \epsilon$ and $s_2^2 + \cdots + s_m^2 \leq 1 - t_0^2 \leq 1/2$
\[
\|\nabla \pi_\gamma(s)\|_2^2 \leq \frac{\gamma^2 (s_2^2 + \cdots + s_m^2)^2 + 2 \gamma^2 s_1^2 (s_2^2 + \cdots + s_m^2)}{(\gamma^2 s_1^2 + s_2^2 + \cdots + s_m^2)^3} \leq \frac{\gamma^2/2}{(\gamma s_2^2 + s_2^2 + \cdots + s_m^2)^3} \leq \frac{1}{2\gamma s_1^6}.
\]
Therefore
\[
|\pi_\gamma(\sigma) - \pi_\gamma(\tilde{\sigma})| \leq \|\nabla \pi_\gamma\|_2 \cdot \|\sigma - \tilde{\sigma}\|_2 \leq \frac{\epsilon}{\sqrt{2\gamma s_1^3}} \leq 2\epsilon.
\]

As the signs of the singular vectors can be chosen arbitrarily, we can assume without loss of generality that $\langle u_1, \tilde{u}_1 \rangle \geq 0$. Together with (3.59) and (3.60) we obtain $\|u_1 - \tilde{u}_1\|_2 \leq \frac{2\epsilon}{\kappa}$ and the same holds also for $\|v_1 - \tilde{v}_1\|_2$. Therefore, we may estimate the difference of the first singular value components by
\[
\|u_1 \pi_\gamma(\sigma)v_1^T - \tilde{u}_1 \pi_\gamma(\tilde{\sigma})\tilde{v}_1^T\|_F \leq \|(u_1 - \tilde{u}_1) \pi_\gamma(\sigma)v_1^T\|_F + \|\tilde{u}_1 (\pi_\gamma(\sigma) - \pi_\gamma(\tilde{\sigma}))v_1^T\|_F + \|\tilde{u}_1 (\pi_\gamma(\tilde{\sigma}) - \pi_\gamma(\tilde{\sigma}))v_1^T\|_F \leq 2\epsilon + \|u_1 - \tilde{u}_1\|_2 + |\pi_\gamma(\sigma) - \pi_\gamma(\tilde{\sigma})| + \|v_1 - \tilde{v}_1\|_2 \leq 2\epsilon + 2\epsilon/\kappa \leq 2^{3/2} \epsilon + 4\epsilon/\kappa.
\] (3.61)

We now need to estimate the difference of the other components of the singular value decomposition. Now notice that
\[
\left\| \sum_{j=1}^k y_j \tilde{z}_j^T \right\|_F^2 = \sum_{j=1}^k \|y_j\|_2^2
\] (3.62)
for arbitrary vectors \( \{y_1, \ldots, y_k\} \subset \mathbb{R}^m \) and orthonormal vectors \( \{z_1, \ldots, z_k\} \subset \mathbb{R}^m \). By applying the triangle inequality and (3.62)

\[
\left\| \sum_{j=2}^{m} u_j \frac{\sigma_j}{\sqrt{\gamma^2 \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_m^2}} v_j^T - \sum_{j=2}^{m} u_j \frac{\tilde{\sigma}_j}{\sqrt{\gamma^2 \tilde{\sigma}_1^2 + \tilde{\sigma}_2^2 + \cdots + \tilde{\sigma}_m^2}} \tilde{v}_j^T \right\|_F \\
\leq \left\| \sum_{j=2}^{m} u_j \frac{\sigma_j}{\sqrt{\gamma^2 \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_m^2}} v_j^T \right\|_F + \left\| \sum_{j=2}^{m} u_j \frac{\tilde{\sigma}_j}{\sqrt{\gamma^2 \tilde{\sigma}_1^2 + \tilde{\sigma}_2^2 + \cdots + \tilde{\sigma}_m^2}} \tilde{v}_j^T \right\|_F \\
= \left( \sum_{j=2}^{m} \frac{\sigma_j^2}{\gamma^2 \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_m^2} \right)^{1/2} + \left( \sum_{j=2}^{m} \frac{\tilde{\sigma}_j^2}{\gamma^2 \tilde{\sigma}_1^2 + \tilde{\sigma}_2^2 + \cdots + \tilde{\sigma}_m^2} \right)^{1/2} \\
\leq \left( \frac{1 - t_0^2}{\gamma^2 t_0^2} \right)^{1/2} + \left( \frac{1 - (t_0 - \epsilon)^2}{\gamma^2 (t_0 - \epsilon)^2} \right)^{1/2} \leq 2 \sqrt{1 - (t_0 - \epsilon)^2} \frac{1}{\gamma (t_0 - \epsilon)} \leq 2 \frac{1}{\sqrt{1 - u^2}} \leq 2 \sqrt{1 - u} \quad \text{for } 1 > u > 1/\sqrt{2}. \tag{3.63}
\]

as \( t_0 - \epsilon > 1/\sqrt{2} \) and \( \frac{1 - u^2}{u} \leq 2 \sqrt{1 - u} \). The statement now follows by adding (3.61) and (3.63).

**Theorem 3.16.** Assume for that \( \|P_A - P_A\|_{F \rightarrow F} < \epsilon < 1 \) and that \( a_1, \ldots, a_m \) are orthonormal. Let \( \|X^0\|_{\infty} > \max \{ \frac{1}{\sqrt{\gamma^2 - 1}}, \frac{1}{\sqrt{2}} + \epsilon + \xi \} \) and \( \sqrt{2} < \gamma \). Then for the iterations \( (X^\ell)_{\ell \in \mathbb{N}} \) produced by Algorithm 3.4, there exists \( \mu_0 < 1 \) such that

\[
\limsup_{\ell \to \infty} |1 - \|X^\ell\|_{\infty}| \leq \frac{\mu_1(\gamma, t_0, \epsilon) + 2\epsilon}{1 - \mu_0} + \epsilon,
\]

where \( \mu_1(\gamma, t_0, \epsilon) \) is as in Lemma 3.15. The sequence \( (X^\ell)_{\ell \in \mathbb{N}} \) is bounded and its accumulation points \( X \) satisfy simultaneously the following properties

\[
\|X\|_F \leq 1 \quad \text{and} \quad \|X\|_{\infty} \geq 1 - \frac{\mu_1(\gamma, t_0, \epsilon) + 2\epsilon}{1 - \mu_0} - \epsilon,
\]

and

\[
\|P_A X\|_F \leq 1 \quad \text{and} \quad \|P_A X\|_{\infty} \geq 1 - \frac{\mu_1(\gamma, t_0, \epsilon) + 2\epsilon}{1 - \mu_0} - 2\epsilon.
\]

**Proof.** We denote the singular value decomposition of \( X^\ell \) by \( X^\ell = \sum_{j=1}^{m} \sigma^\ell u_j^\ell \otimes v_j^\ell \) and the one of \( P_A X^\ell \) by \( P_A X^\ell = \sum_{j=1}^{m} \sigma^\ell a_j^\ell \otimes \tilde{v}_j^\ell \), where \( i_j \) is a suitable rearrangement of the index set \( \{1, \ldots, m\} \). By Lemma 3.15 we can further develop the following estimates:

\[
\epsilon + \sigma_1^{\ell+1} \geq \|X^{\ell+1}\|_{\infty} = \|P_A \Pi_\gamma (X^{\ell})\|_{\infty} \geq \|P_A \Pi_\gamma (X^{\ell})\|_{\infty} - \|(P_A - P_A) \Pi_\gamma (X^{\ell})\|_{\infty} \geq \|P_A \Pi_\gamma (X^{\ell})\|_{\infty} - \|(P_A - P_A) \Pi_\gamma (X^{\ell})\|_F \geq \|P_A \Pi_\gamma (P_A X^{\ell})\|_{\infty} - \epsilon = \|P_A \Pi_\gamma (P_A X^{\ell}) + P_A \Pi_\gamma (P_A X^{\ell}) - P_A \Pi_\gamma (P_A X^{\ell})\|_{\infty} - \epsilon \geq \|P_A \Pi_\gamma (P_A X^{\ell})\|_{\infty} - \Pi_\gamma (P_A X^{\ell})\|_F - \epsilon \geq \frac{\gamma \sigma_1^\ell}{\sqrt{(\gamma^2 - 1)\sigma_1^2 + 1}} - \mu_1(\gamma, t_0, \epsilon) - \epsilon.
\]
Hence, we obtain

\[ 1 - \sigma_{1}^{\ell+1} \leq 1 - \frac{\gamma \sigma_{1}^{\ell}}{\sqrt{(\gamma^2 - 1)\sigma_{1}^{\ell2} + 1}} + \mu_1(\gamma, t_0, \epsilon) + 2\epsilon. \]

By an estimate similar to (3.57) and following the arguments given before, we conclude that

\[ 1 - \sigma_{1}^{\ell+1} \leq \mu_0(1 - \sigma_{1}^{\ell}) + \eta_0, \quad (3.64) \]

where \( \eta_0 = \mu_1(\gamma, t_0, \epsilon) + 2\epsilon \). As \( X^\ell = P_A \Pi_\gamma(X^{\ell-1}) \) and \( P_A \) and \( P_{\tilde{A}} \) are orthogonal projections we have that

\[ \sigma_{1}^{\ell} \leq \|P_A X^\ell\|_F \leq \|X^\ell\|_F \leq \|\Pi_\gamma(X^{\ell-1})\|_F = 1. \]

Hence, actually, the recursion (3.64) can be rewritten as

\[ |1 - \sigma_{1}^{\ell+1}| \leq \mu_0 |1 - \sigma_{1}^{\ell}| + \eta_0 \]

\[ \leq \mu_0^{\ell+1} |1 - \sigma_{1}^{0}| + \eta_0 \sum_{k=0}^{\ell} \mu_0^k. \]

This implies

\[ \limsup_{\ell \to \infty} |1 - \|X^\ell\|_\infty| = \limsup_{\ell \to \infty} |1 - \tilde{\sigma}_{1}^{\ell}| \leq \limsup_{\ell \to \infty} |1 - \sigma_{1}^{\ell}| + \epsilon \leq \eta_0 \frac{1 - \mu_0}{1 - \mu_0} + \epsilon. \quad (3.65) \]

Since the sequence \( (X^\ell)_{\ell} \) is bounded, it has accumulation points \( \bar{X} \), and as a consequence of (3.65) we obtain that \( \bar{X} \) has simultaneously the following properties

\[ \|\bar{X}\|_F \leq 1 \quad \text{and} \quad \|\bar{X}\|_\infty \geq 1 - \frac{\eta_0}{1 - \mu_0} - \epsilon, \]

and

\[ \|P_A \bar{X}\|_F \leq 1 \quad \text{and} \quad \|P_A \bar{X}\|_\infty \geq 1 - \frac{\eta_0}{1 - \mu_0} - 2\epsilon. \]

\[ \square \]

**Remark 9.** Given the singular value decompositions \( \bar{X} = \sum_{j=1}^{m} \bar{\sigma}_j \bar{\sigma}_j \otimes \bar{\sigma}_j \) and \( P_A \bar{X} = \sum_{j=1}^{m} \sigma_{j}^\infty a_j \otimes a_j \), by applying again Wedin’s bound we obtain that, for instance

\[ \|\bar{v}_1 \otimes \bar{v}_1 - a_{i_1} \otimes a_{i_1}\|_F \leq \frac{2}{1 - \frac{\eta_0}{1 - \mu_0} + \epsilon - \sqrt{1 - (1 - \frac{\eta_0}{1 - \mu_0})^2}}. \]

Notice that for \( \epsilon \to 0 \) we obtain \( \eta_0 = \mu_1(\gamma, t_0, \epsilon) + 2\epsilon \to 2\sqrt{1 - t_0}. \)

### 4 Approximating the sum of ridge functions

The main aim of our work is to identify the structure of functions, which take the form of (1.2). Nevertheless, once the ridge directions \( a_j \) are identified or approximated, we can produce also a uniform approximation of \( f \).
Before we come to that we clarify one technical issue of (1.2). It is easy to see, that the representation (1.2) is not unique due to the free choice of additive factors. Indeed, if we add to the profiles \((g_j)_{j=1}^m\) arbitrary constants which sum up to zero, we obtain the same function \(f\). By simply sampling \(f\) at zero and subtracting this value from \(f\), we may assume without loss of generality that \(f(0) = 0\). If \(0 = f(0) = \sum_{i=1}^m g_i(0)\) then \(\{g_i(0) : i = 1, \ldots, m\}\) are indeed constants with zero sum and we can subtract them term by term \(f(x) = \sum_{i=1}^m (g_i(a_i \cdot x) - g_i(0))\). Consequently, we can assume without loss of generality that \(g_1(0) = \cdots = g_m(0) = 0\) \((4.1)\).

For the uniform approximation of \(f\) fulfilling (1.2) and (4.1), let us assume the we run Algorithm 3.4 with different initial values and obtain the approximation of the ridge directions \((a_j)_{j=1}^m\) by unit-norm vectors \((\hat{a}_j)_{j=1}^m\). We then sample \(f\) along the vectors in the dual basis \((\hat{b}_j)_{j=1}^m\) to obtain an approximation of the univariate ridge profiles \(g_1, \ldots, g_m\), which are uniquely determined by (4.1). The approximation \(\hat{f}\) of \(f\) is then obtained by putting all these ingredients together. The resulting algorithm and the analysis of its performance are as described below.

**Algorithm 4.1.**

- Let \(\hat{a}_j\) be the normalized approximations of \(a_j, j = 1, \ldots, m\).
- Let \((\hat{b}_j)_{j=1}^m\) be the dual basis to \((\hat{a}_j)_{j=1}^m\).
- Put \(\hat{g}_j(t) := f(t \hat{b}_j), t \in (-1/\|\hat{b}_j\|_2, 1/\|\hat{b}_j\|_2)\).
- Put \(\hat{f}(x) := \sum_{j=1}^m \hat{g}_j(\hat{a}_j \cdot x), \|x\|_2 \leq 1\).

**Theorem 4.1.** Let \(S(a_1, \ldots, a_m) \leq \varepsilon, S(\hat{a}_1, \ldots, \hat{a}_m) \leq \varepsilon',\) and \(\left(\sum_{j=1}^m \|a_j - \hat{a}_j\|^2_2\right)^{1/2} \leq \eta\). Then \(\hat{f}\) constructed by Algorithm 4.1 satisfies

\[\|f - \hat{f}\|_\infty \leq 5C_2(1 + \xi(\varepsilon, \varepsilon')) \max(\eta, \eta^2),\]

where \(\xi(\varepsilon, \varepsilon') \to 0\) if \((\varepsilon, \varepsilon') \to (0, 0)\).

**Proof.** We use that \(g_i(0) = 0\) for \(i = 1, \ldots, m\), \(a_i \cdot x = \sum_j (\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot a_i)\), Taylor’s formula,
and estimate for $x \in \mathbb{R}^m$ with $\|x\|_2 \leq 1$

\[
|f(x) - \tilde{f}(x)| = \left| \sum_{i=1}^{m} g_i(a_i \cdot x) - \sum_{j=1}^{m} \hat{g}_j(\hat{a}_j \cdot x) \right| = \left| \sum_{i=1}^{m} g_i(a_i \cdot x) - \sum_{j=1}^{m} f(\hat{a}_j \cdot x) \hat{b}_j \right|
\]

\[
= \left| \sum_{i=1}^{m} g_i(a_i \cdot x) - \sum_{j=1}^{m} \sum_{i=1}^{m} g_i((\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot a_i)) \right|
\]

\[
\leq \sum_{i=1}^{m} \left| g_i(a_i \cdot x) - \sum_{j=1}^{m} g_i((\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot a_i)) \right|
\]

\[
= \sum_{i=1}^{m} \left| g_i(0) a_i \cdot x - \sum_{j=1}^{m} g_i(0) (\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot a_i) \right|
\]

\[
+ \int_0^{a_i \cdot x} (a_i \cdot x - u) g_i''(u) du - \sum_{j=1}^{m} \int_0^{(\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot a_i)} ((\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot a_i) - u) g_i''(u) du
\]

\[
\leq \sum_{i=1}^{m} \int_0^{a_i \cdot x} (a_i \cdot x - u) g_i''(u) du - \int_0^{(\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot a_i)} ((\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot a_i) - u) g_i''(u) du
\]

\[
+ \sum_{i=1}^{m} \sum_{j \neq i} \int_0^{(\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot a_i - \hat{a}_i)} ((\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot (a_i - \hat{a}_i)) - u) g_i''(u) du
\]

\[
= I + II.
\]

We use Lemma 6.1 and Lemma 6.3 to bound the first term by

\[
I \leq C_2 \sum_{i=1}^{m} \left\{ |a_i \cdot x| \cdot |a_i \cdot x - (\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot a_i)| + |a_i \cdot x - (\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot a_i)|^2 \right\} / 2
\]

\[
\leq C_2 \left( \sum_{i=1}^{m} |a_i \cdot x|^2 \right)^{1/2} \cdot \left( \sum_{i=1}^{m} |a_i \cdot x - (\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot a_i)|^2 \right)^{1/2}
\]

\[
+ \frac{C_2}{2} \sum_{i=1}^{m} |a_i \cdot x - (\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot a_i)|^2 = I' + I'',
\]

where

\[
I' \leq C_2 (1 + \varepsilon) \cdot \left( \sum_{i=1}^{m} |(a_i - \hat{a}_i) \cdot x|^2 \right)^{1/2} + \left( \sum_{i=1}^{m} |(\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot (\hat{a}_i - \hat{a}_i))|^2 \right)^{1/2}
\]

\[
\leq C_2 (1 + \varepsilon) \eta + C_2 (1 + \varepsilon) \max_j \|\hat{b}_j\|_2 \eta
\]

and

\[
I'' \leq C_2 \sum_{i=1}^{m} \left( |(a_i - \hat{a}_i) \cdot x|^2 + |(\hat{a}_i \cdot x) \cdot (\hat{b}_i \cdot (\hat{a}_i - \hat{a}_i))|^2 \right)
\]

\[
\leq C_2 \eta^2 + C_2 \max_j \|\hat{b}_j\|^2_2 \eta^2.
\]
Next, we estimate the second term by

$$II \leq C_2 \sum_{i=1}^{m} \sum_{j=1}^{m} |(\hat{a}_j \cdot x) \cdot (\hat{b}_j \cdot (a_i - \hat{a}_i))|^2 \leq C_2 \sum_{i,j=1}^{m} (\hat{a}_j \cdot x)^2 \cdot \|\hat{b}_j\|_2^2 \cdot \|a_i - \hat{a}_i\|_2^2$$

$$\leq C_2 \max_j \|\hat{b}_j\|_2^2 \cdot \sum_{j=1}^{m} (\hat{a}_j \cdot x)^2 \cdot \sum_{i=1}^{m} \|a_i - \hat{a}_i\|_2^2 \leq C_2 \max_j \|\hat{b}_j\|_2^2 \cdot (1 + \varepsilon')^2 \eta^2.$$ 

Using Lemma 6.3 (vi) and summing up these estimates we get

$$\|f - \hat{f}\|_\infty \leq 5C_2(1 + \Xi(\varepsilon, \varepsilon')) \max(\eta, \eta^2),$$

where $\Xi(\varepsilon, \varepsilon') \to 0$ if $(\varepsilon, \varepsilon') \to (0,0)$.

**Remark 10.** By triangle inequality, the parameters $\varepsilon, \varepsilon'$ and $\eta$ from Theorem 4.1 satisfy $\varepsilon' \leq \varepsilon + \eta$.

## 5 Numerical experiments

In this section we demonstrate numerically the efficiency of the pipeline of the algorithms we analyzed in the previous sections for the robust identification of the weights of a network written in compact form as $f(x) = b^T g(A^T x + \theta)$ of $m$ nodes in dimension $m$, where $A \in \mathbb{R}^{m \times m}, b, \theta \in \mathbb{R}^m$. Throughout the experiments we use networks with random configurations. To generate a random network we specify $m$ and $\varepsilon$, which is the degree of near orthogonality of $A$ and sample the remaining parameters as

- $A$: First we draw an orthogonal $m \times m$ matrix from the Haar distribution. Then we proceed iterating the following adjustments: we perturb the singular values by Gaussian noise with a given variance, then normalize the columns, and we check whether $A$ has reached the desired degree $\varepsilon$ of near-orthonormality up to a tolerance of $\pm 0.001$; if this does not occur, then we modify the variance of the Gaussian noise in a bisection fashion to search iteratively the right level of near-orthonormality;
- $b = (b_1, \ldots, b_m)^T$ with $b_i \sim \mathcal{N}(1, 1/5)$ selected independently;
- $\theta = (\theta_1, \ldots, \theta_m)$ with $\theta_i \sim \mathcal{N}(0, 1/5)$ selected independently;
- $g(t) = \tanh(t)$.

This setting corresponds to (1.2) with $g_i(t) = b_i \tanh(t + \theta_i)$.

### 5.1 Exact weight identification

We will consider below trials for $m = 20$. The choice of a small dimension is simply due to the necessity of running in a reasonable time a large number of trials to estimate the empirical probability of success, but the algorithms can comfortably be implemented in higher dimensions $m \approx 10^3$ on a Laptop. In this case the memory needed for storing 64 bit floating point matrices $Y$ as appearing in Algorithm 2.1-Algorithm 3.1 is given by $m^2 \times m \times 8$ bytes $\approx 8$GB. For much higher dimensions the use of HPC is needed, see Section 5.2 and Section 5.3 below.
Denote by $a_1, \ldots, a_m$ the columns of $A$. As clarified by Theorem 4.1 the fundamental issue is in fact the robust identification of the network weights $a_i$, while the identification of the rest of the network is its direct consequence. For the sake of simplicity, we present here results based on active sampling. Accordingly, we denote with $m_X$ the number of sampled Hessians of the function $f$, which are computed by finite difference approximations with stepsize $0.001$, cf. (3.2). For each pair $(m_X, \varepsilon)$ of number of Hessians and near-orthonormality level, we run 60 trials. In each of the trials we first construct the subspace $\tilde{A}$ by Algorithm 3.1 and then try to compute all $m = 20$ vectors $a_1, \ldots, a_m$ by applying Algorithm 3.4 repeatedly. One run of Algorithm 3.1 returns at random one of the $a_i$, therefore we need to run the algorithm at least $m$ times to have a chance of recovering all the vectors. For the hyperparameter of number of repetitions we choose $n_{\text{rep}} = 180$. In each of the $n_{\text{rep}}$ repetitions we carried out 100 steps of the algorithm with $\gamma = 2$ and we used this number of steps as a stopping criterion. For each of the 60 trials we get $180$ vectors $V = \{v_1, \ldots, v_{\text{rep}}\}$. In our numerical experiments $V$ always contained only approximations to (some or all) original vectors $a_i$ and no spurious cases seem ever occurring. For a given tolerance $\tau$ we measure the number of well-approximated vectors as

$$n_{\text{found}} := \# \{ i \in [m] : \min \{ \|v + a_i\|_2, \|v - a_i\|_2 \} \leq \delta \text{ for any } v \in V \},$$

and we set $\delta = 0.05$ in our experiments. Figure 4 shows the ratio of the number of trials where $n_{\text{found}} = m$ for different degrees of near-orthonormality and amounts of approximated Hessians. From the figure, it is clear that our pipeline of the algorithms is able to reconstruct exactly all $m = 20$ network weights $a_1, \ldots, a_m$ with high probability with a number $m_X \approx m = 20$ of sampled Hessians, which is the information theoretical lower bound. Moreover, as shown in Figure 4, exact recovery is obtained also for levels $\varepsilon > 1$ of near-orthonormality. Even for $\varepsilon \approx 3$ the algorithm recovers all vectors with overwhelming (empirical) probability. This numerical evidence suggests that the $\varepsilon$-quasi-orthonormality is a quite conservative measure of separation of the vectors $a_1, \ldots, a_m$ and that in practice it is sufficient that they are enough separated and a near orthogonality is not necessary.

Figure 4: Phase transition diagram displaying the empirical success probability of recovering all the vectors $a_1, \ldots, a_m$ for a given number $m_X$ of sampled Hessians and near-orthonormality level $\varepsilon$ of the searched vectors.
5.2 Exploring computational time

The previous section indicates that having around $m_X \approx m$ (approximated) Hessians is sufficient for recovery. We use the parameters above and explore how much computational time different blocks of the algorithm pipeline need for increasing dimensionalities $m = m_X$. Additionally, we keep the deviation from an orthonormal system constant at $\varepsilon = 1$ (which should not have much influence on the runtime anyway). We split the algorithm into three stages: the sampling and approximation of the Hessians, the realization of Algorithm 3.1 (which below we denote PCA), and finally the search of the rank-1 matrices by Algorithm 3.4. For the last stage we only measure the time needed to find one rank-1 matrix. Additionally we also track one version where we replace the SVD in stage 2 (Algorithm 3.1) by a randomized SVD [26]. The computational times of the different phases are plotted in Figure 5. As a clear disclaimer, let us stress that our computational time figures are relative to quite straightforward off the books implementations, with no particular tuning or optimization whatsoever. Hence, they should not be taken as a reference of the absolute performance of our algorithmic pipeline, rather as an illustration of our theoretical findings and an indication of feasibility, even with relatively modest computational resources. In fact, we expect that careful and optimized coding and parallelization will yield tremendous speed-ups and more efficient memory usage over the presented figures.

As mentioned above, we need to apply Algorithm 3.4 repeatedly to find all the weights $a_i$. An interesting question is how many times $n_{\text{rep}}$ do we need to repeat Algorithm 3.4 with random initial iteration to be able to compute all the weights. If we assume a uniform distribution for Algorithm 3.4 to compute at random one of the weights, then our problem is equivalent to the classical coupon collector’s problem. A well known result from probability [32, Section 8.4] tells us that we need on average

$$E[n_{\text{rep}}] = m \ln m + \gamma m + \frac{1}{2} + O(1/m)$$

(5.1)

repetitions to cover all vectors, where $\gamma \approx 0.57721\ldots$ is the Euler-Mascheroni constant. Large deviation bounds are also available, see, e.g., [21]. Using this as a baseline to measure the cost of the algorithm yields the cumulative results in Figure 6. It is important to notice that the showed runtime as well as the memory consumption (next section) depend heavily on the implementation, which was not extensively optimized with respect to both. However, even with this in mind, it is painfully obvious that finding a way to avoid Algorithm 3.4 picking duplicate vectors would make the algorithm much more efficient. Nevertheless, it is also clear that the procedure can be easily parallelized, using ca. $E[N_{\text{rep}}]$ (5.1) processors.

5.3 Exploring memory allocation

As previously, we split the algorithm into three stages and measure the consumed memory of the process for $m = 100$ and $m = 125$ (cf. Figure 7-8). The most expensive part is clearly the PCA (Algorithm 3.1). However, choosing a randomized SVD variant required only 50% of the memory in our example, without diminishing significantly accuracy. This stage needs to be further optimized with respect to memory in the future, including considering lower bit encoding etc.
5.4 Comparison to gradient descent

A popular method for training a neural network is minimizing the misfit (here we consider the mean squared error) on the output of the network over a large number of inputs by means of gradient descent. In this section we would like to compare the behavior of our pipeline of algorithms with gradient descent we choose the same setting for both approaches. In particular, we assume that every other parameter of the network except the (inner) weights $a_1, \ldots, a_m$ is known and fixed. To be precise:

- We assume $b, \theta$ are known and fixed;
Figure 7: Memory consumption for $m = 100$. Classical SVD (top), randomized SVD (bottom). The dashed red lines indicates the cartesian coordinates (time × memory) of the memory peak.

- We set $m = 20$ and $\varepsilon = 1$ (i.e. $a_1, \ldots, a_m$ will be $\varepsilon$-nearly-orthonormal);

- For each random network we run our method for gradually increasing number of sampled approximated Hessians and with $n_{rep}$ sufficiently large. From the resulting vectors we compute $\hat{a}_1, \ldots, \hat{a}_m$ by clustering them by $k$-means. Finally we record the error of the new network where $A$ is substituted with our estimate $\hat{A}$ on a completely new set of $10^5$ datapoints generated at random uniformly on $B_d^1$ that were not used during the previous steps. The error is measured via mean square error (MSE/$L^2$-squared) / uniform norm and we record the distance of the estimated $\hat{A}$ to $A$ in the Frobenius norm.

- We emulate the same procedure by using gradient descent to minimize the MSE misfit over the same training datapoints. Approximating one Hessian by finite-differences requires $1 + \frac{d^2 + d}{2}$ samples. The stepsize of gradient descent method remains fixed at 0.1 and we do exactly 1000 steps for each trial.
We average everything over 10 random trial networks, the results are collected in Figure 9 and Figure 10.

On the one hand, gradient descent seems to require only a very small amount of samples (≈ 50, see the right plot in Figure 10) to converge against a very efficient local minimum representing a good approximation of the network in MSE, whereas our algorithm requires at least $m$ Hessians. However, the generated network by gradient descent is not optimal as one can observe from the non-vanishing uniform norm approximation, see the right plot in Figure 9. On the other hand, if we have enough Hessians, then our method returns the optimal network with vanishing uniform norm discrepancy. Additionally, gradient descent will never come close to the original weight matrix $A$, while our algorithm is able to consistently recover a very good approximation of $A$, see the left plot in Figure 10.
Figure 9: Average approximation error of 10 random networks with $m = 20, \varepsilon = 1$ in terms of MSE (left), uniform norm (right). The errors were measured over $10^5$ datapoints generated uniform at random on the ball $B_1^d$.

Figure 10: Approximation error of $A$ in the Frobenius norm (left). Approximation error of gradient descent for 1-200 samples (right).

6 Appendix

We collect several technical tools needed throughout the paper. We start with an auxiliary lemma, which can be easily verified by a straightforward calculation.

**Lemma 6.1.** Let $I \subset \mathbb{R}$ be an interval containing zero and let $G : I \to \mathbb{R}$ be measurable. Then for any $x, y \in I$

$$\left| \int_0^x (x-u)G(u)du - \int_0^y (y-u)G(u)du \right| \leq \max_{u \in I} |G(u)| \cdot \left( |x| \cdot |y-x| + |y-x|^2/2 \right).$$

6.1 Nearly orthonormal vectors

In this section we discuss some basic properties of the notion of $\varepsilon$-nearly-orthonormal vectors, cf. Definition 1.1. There we defined the quantity $S(a_1, \ldots, a_m)$ for vectors $a_1, \ldots, a_m$, which have unit norm. With a slight abuse of notation, we extend the definition also to the
case, where $a_i$’s are not normalized, i.e. we define

$$S(\alpha_1, \ldots, \alpha_m) = \inf\left\{ \left( \sum_{i=1}^{m} \|\alpha_i - w_i\|_2^2 \right)^{1/2} : w_1, \ldots, w_m \text{ orthonormal basis in } \mathbb{R}^m \right\}$$

for every set $\{\alpha_1, \ldots, \alpha_m\} \subset \mathbb{R}^m$.

**Theorem 6.2.** (i) Let $a_1, \ldots, a_m \in \mathbb{R}^m$ and let $A \in \mathbb{R}^{m \times m}$ be a matrix with columns $a_1, \ldots, a_m$. Then

$$S(a_1, \ldots, a_m) = \left( \sum_{i=1}^{m} (\sigma_i - 1)^2 \right)^{1/2}, \quad (6.1)$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$ are the singular values of $A$.

(ii) Furthermore,

$$S(a_1, \ldots, a_m) \leq \|AA^T - I_m\|_F \leq (\|A\| + 1)S(a_1, \ldots, a_m).$$

**Proof.** (i) The result is very well known and the proof follows easily by singular value decomposition of $A = U\Sigma V^T$. The closest orthogonal basis $w_1, \ldots, w_m$ is given as the columns of the matrix $W = UV^T$.

(ii) First observe that if $A = U\Sigma V^T$, then

$$\|AA^T - I_m\|_F = \|U\Sigma^2 U^T - I_m\|_F = \left( \sum_{i=1}^{m} [\sigma_i^2 - 1]^2 \right)^{1/2}.$$ 

Hence

$$S(a_1, \ldots, a_m) = \left( \sum_{i=1}^{m} (\sigma_i - 1)^2 \right)^{1/2} \leq \left( \sum_{i=1}^{m} (\sigma_i - 1)^2 (\sigma_i + 1)^2 \right)^{1/2}$$

$$= \left( \sum_{i=1}^{m} (\sigma_i^2 - 1)^2 \right)^{1/2} = \|AA^T - I_m\|_F$$

$$\leq \max_i (\sigma_i + 1) \left( \sum_{i=1}^{m} [\sigma_i - 1]^2 \right)^{1/2} = (\|A\| + 1)S(a_1, \ldots, a_m).$$

**Lemma 6.3.** Let $\varepsilon > 0$ and let $a_1, \ldots, a_m \in \mathbb{R}^m$ with $S(a_1, \ldots, a_m) \leq \varepsilon$ and $\|a_i\|_2 = 1$ for all $i = 1, \ldots, m$ and let $A \in \mathbb{R}^{m \times m}$ be a matrix with columns $a_1, \ldots, a_m$.

(i) Then

$$(1 - \varepsilon)\|y\|_2 \leq \|Ay\|_2 \leq (1 + \varepsilon)\|y\|_2$$

for all $y \in \mathbb{R}^m$. The result holds with identical proof also for $A^T$ instead of $A$ substituted in the inequality.

(ii) Let $M = \sum_{j=1}^{m} \sigma_j a_j \otimes a_j$, then $\|M\|_\infty \leq (1 + \varepsilon)^2 \|\sigma\|_\infty$.

(iii) $\sum_{k \neq j} |\langle a_k, a_j \rangle|^2 \leq 2\varepsilon^2$ for all $j = 1, \ldots, m$.  

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(iv) $S(a_1 \otimes a_1, \ldots, a_m \otimes a_m) \leq 2\varepsilon$.

(v) $(1 - 2\varepsilon)\|\sigma\|_2 \leq \| \sum_{j=1}^{m} \sigma_j a_j \otimes a_j \|_F \leq (1 + 2\varepsilon)\|\sigma\|_2$. 

(vi) Let $b_j, j = 1, \ldots, m$ be the dual basis of $a_j, j = 1, \ldots, m$ (i.e. $\langle b_i, a_j \rangle = \delta_{i,j}$). Then $\|b_j\|_2 \leq 1/(1 - \varepsilon)$ for all $j = 1, \ldots, m$.

**Proof.**  (i) Let $W$ be the optimal orthonormal matrix for $A$. Then 

$$\|Ay\|_2 = \|(A - W)y + Wy\|_2 \leq \|A - W\|_\infty \cdot \|y\|_2 + \|Wy\|_2 \leq (1 + \varepsilon)\|y\|_2.$$ 

The other estimate from below follows by applying the inverse triangle inequality. The proof can be used similarly also for obtaining the bounds for $A^T$ instead of $A$.

(ii) We estimate by (i)

$$\|M\|_\infty = \sup_{x: \|x\|_2 \leq 1} |\langle x, Mx \rangle| \leq \sup_{x: \|x\|_2 \leq 1} \sum_{j=1}^{m} |\sigma_j| \cdot |\langle a_j, x \rangle|^2$$

$$\leq \|\sigma\|_\infty \cdot \sup_{x: \|x\|_2 \leq 1} \sum_{j=1}^{m} |\langle a_j, x \rangle|^2 \leq (1 + \varepsilon)^2 \|\sigma\|_\infty.$$ 

(iii) We get just by triangle inequality and the inequality between the arithmetic and quadratic mean

$$\left( \sum_{k \neq j} |\langle a_k, a_j \rangle|^2 \right)^{1/2} = \left( \sum_{k \neq j} (|\langle a_k - w_k, a_j \rangle|^2 + |\langle w_k, a_j \rangle|^2) \right)^{1/2}$$

$$\leq \left( \sum_{k \neq j} |\langle a_k - w_k, a_j \rangle|^2 \right)^{1/2} + \left( \sum_{k \neq j} |\langle w_k, a_j - w_j \rangle|^2 \right)^{1/2}$$

$$\leq \left( \sum_{k \neq j} \|a_k - w_k\|_2^2 \cdot \|a_j\|_2^2 \right)^{1/2} + \|a_j - w_j\|_2$$

$$\leq \sqrt{2} \left( \|a_j - w_j\|_2^2 + \sum_{k \neq j} \|a_k - w_k\|_2^2 \right)^{1/2} \leq \sqrt{2} \varepsilon.$$ 

(iv) The result follows by

$$\left( \sum_{j=1}^{m} \|a_j \otimes a_j - w_j \otimes w_j\|_F^2 \right)^{1/2} = \left( \sum_{j=1}^{m} \|a_j \otimes (a_j - w_j) + (a_j - w_j) \otimes w_j\|_F^2 \right)^{1/2}$$

$$\leq \left( \sum_{j=1}^{m} \|a_j \otimes (a_j - w_j)\|_F^2 \right)^{1/2} + \left( \sum_{j=1}^{m} \|(a_j - w_j) \otimes w_j\|_F^2 \right)^{1/2}$$

$$= \left( \sum_{j=1}^{m} \|a_j - w_j\|_2^2 \cdot \|a_j\|_2^2 \right)^{1/2} + \left( \sum_{j=1}^{m} \|a_j - w_j\|_2^2 \cdot \|w_j\|_2^2 \right)^{1/2} \leq 2\varepsilon.$$ 

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(v) Using (iv) we obtain
\[
\left\| \sum_{j=1}^{m} \sigma_j a_j \otimes a_j \right\|_F \leq \left\| \sum_{j=1}^{m} \sigma_j (a_j \otimes a_j - w_j \otimes w_j) \right\|_F + \left\| \sum_{j=1}^{m} \sigma_j w_j \otimes w_j \right\|_F \\
\leq \|\sigma\|_2 + \sum_{j=1}^{m} |\sigma_j| \cdot \|a_j \otimes a_j - w_j \otimes w_j\|_F \\
\leq \|\sigma\|_2 + \left( \sum_{j=1}^{m} \sigma_j^2 \right)^{1/2} \cdot \left( \sum_{j=1}^{m} \|a_j \otimes a_j - w_j \otimes w_j\|_F^2 \right)^{1/2} \\
\leq (1 + 2\varepsilon)\|\sigma\|_2
\]
and similarly for the other side.

(vi) Using the definition of \( S(a_1, \ldots, a_m) \), we obtain for the optimal orthonormal basis \( w_1, \ldots, w_m \)
\[
\|b_j\|_2 = \left( \sum_{k=1}^{m} (b_j, w_k)^2 \right)^{1/2} = \left( \sum_{k=1}^{m} [(b_j, a_k) + (b_j, w_k - a_k)]^2 \right)^{1/2} \\
\leq \left( \sum_{k=1}^{m} (b_j, a_k)^2 \right)^{1/2} + \left( \sum_{k=1}^{m} (b_j, w_k - a_k)^2 \right)^{1/2} \\
\leq 1 + \left( \sum_{k=1}^{m} \|b_j\|_2^2 \cdot \|w_k - a_k\|_2^2 \right)^{1/2} \leq 1 + \varepsilon \|b_j\|_2.
\]

The next lemma shows that normalization of a set of vectors does not influence much their distance to an orthonormal basis.

**Lemma 6.4.** Let \( \{\alpha_1, \ldots, \alpha_m\} \subset \mathbb{R}^m \) be arbitrary non-zero vectors in \( \mathbb{R}^m \). Then
\[
S\left( \frac{\alpha_1}{\|\alpha_1\|_2}, \ldots, \frac{\alpha_m}{\|\alpha_m\|_2} \right) \leq \sqrt{2} S(\alpha_1, \ldots, \alpha_m).
\]

**Proof.** Let \( \{w_1, \ldots, w_m\} \subset \mathbb{R}^m \) be the closest orthonormal basis to \( \alpha_1, \ldots, \alpha_m \). Then we may assume that \( \langle \alpha_i, w_i \rangle \geq 0 \), otherwise exchanging \( w_i \) for \( -w_i \) would decrease the distance to \( \{\alpha_1, \ldots, \alpha_m\} \).

For every \( i = 1, \ldots, m \), we obtain
\[
\|\alpha_i - w_i\|_2^2 \geq \left\| \left\langle w_i, \frac{\alpha_i}{\|\alpha_i\|_2} \right\rangle \frac{\alpha_i}{\|\alpha_i\|_2} - w_i \right\|_2^2 = 1 - \left\langle w_i, \frac{\alpha_i}{\|\alpha_i\|_2} \right\rangle^2
\]
and therefore
\[
\left\| \frac{\alpha_i}{\|\alpha_i\|_2} - w_i \right\|_2^2 = 2 \left( 1 - \left\langle \frac{\alpha_i}{\|\alpha_i\|_2}, w_i \right\rangle \right) \leq 2 \left( 1 - \frac{(\alpha_i, w_i)^2}{\|\alpha_i\|_2^2} \right) \leq 2 \|\alpha_i - w_i\|_2^2.
\]
To finish the proof, we sum up over \( i = 1, \ldots, m \) and take the square root. \( \square \)
Lemma 6.5. Let \( \{\alpha_1, \ldots, \alpha_m\} \subset \mathbb{R}^n \) be arbitrary linearly independent vectors with unit Euclidean norm and let \( \{\omega_1, \ldots, \omega_m\} \subset \mathbb{R}^n \) be orthonormal. Let \( A = \text{span}\{\alpha_1, \ldots, \alpha_m\} \), \( \hat{A} = \text{span}\{\omega_1, \ldots, \omega_m\} \), and
\[
\left( \sum_{i=1}^m \|\alpha_i - \omega_i\|_2^2 \right)^{1/2} \leq \varepsilon < 1.
\]
Then
\[
\|P_A - P_{\hat{A}}\|_\infty \leq 5\varepsilon,
\]
where \( P_A \) and \( P_{\hat{A}} \) are the orthogonal projections on \( A \) and \( \hat{A} \) respectively, and the norm \( \|\cdot\|_\infty \) represents the operator norm for operators on the Euclidean space \( \mathbb{R}^n \).

Proof. Let \( A \in \mathbb{R}^{n \times m} \) have columns \( \alpha_1, \ldots, \alpha_m \) and let \( W \in \mathbb{R}^{n \times m} \) have columns \( \omega_1, \ldots, \omega_m \). Then \( P_{\hat{A}} = WW^T \). If \( A = U \Sigma V^T \) is the singular value decomposition of \( A \) with \( U \in \mathbb{R}^{n \times m} \) and \( V \in \mathbb{R}^{m \times m} \), then \( P_A = UU^T \). Using \( U \Sigma = AV \), we then obtain for \( \|\cdot\| = \|\cdot\|_\infty \)
\[
\|P_A - P_{\hat{A}}\| = \|UU^T - WW^T\| = \|UU^T - (U \Sigma)(U \Sigma)^T + (U \Sigma)(U \Sigma)^T - WW^T\|
\leq \|UU^T - USU^2U^T\| + \|AVV^T A^T - WW^T\|
\leq \|I - \Sigma^2\|_2 + \|A(A^T - W^T)\| + \|A - W\|_F
\leq \max_i |1 - \sigma_i^2| + \|A\| \cdot \|A^T - W^T\|_F + \|A - W\|_F
\leq \varepsilon^2 + \varepsilon(1 + \varepsilon) + \varepsilon \leq 4\varepsilon.
\]

6.2 Stability of the singular value decomposition

Given two matrices \( B \) and \( \tilde{B} \) with corresponding singular value decompositions
\[
B = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix}
\]
and
\[
\tilde{B} = \begin{pmatrix} \tilde{U}_1 & \tilde{U}_2 \end{pmatrix} \begin{pmatrix} \tilde{\Sigma}_1 & 0 \\ 0 & \tilde{\Sigma}_2 \end{pmatrix} \begin{pmatrix} \tilde{V}_1^T \\ \tilde{V}_2^T \end{pmatrix},
\]
where it is understood that two corresponding submatrices, e.g., \( U_1, \tilde{U}_1 \), have the same size, we would like to bound the difference between \( V_1 \) and \( \tilde{V}_1 \) by the error \( \|B - \tilde{B}\|_F \). As a consequence of Wedin’s perturbation bound [64], see also [58, Section 7], we have the following useful result.

Theorem 6.6 (Stability of subspaces - Wedin’s bound). If there is an \( \bar{\alpha} > 0 \) such that
\[
\min_{\ell, \tilde{\ell}} |\sigma_{\ell}(\Sigma_1) - \sigma_{\tilde{\ell}}(\Sigma_2)| \geq \bar{\alpha}, \tag{6.2}
\]
and
\[
\min_{\ell} \left|\sigma_{\ell}(\Sigma_1)\right| \geq \bar{\alpha}, \tag{6.3}
\]
\[
\max\{\|\sin(\Theta(U_1, \tilde{U}_1))\|_p, \|\sin(\Theta(V_1, \tilde{V}_1))\|_p\} \leq \frac{1}{\alpha} \|B - \tilde{B}\|_p,
\]
where \(\Theta(V,W)\) is the vector of the principal angles between the subspaces \(V\) and \(W\) and \(\|\cdot\|_p\) is an arbitrary \(p\)-norm or Schatten-\(p\)-norm for \(1 \leq p \leq \infty\). The case of \(p = 2\) corresponds to the Frobenius norm and the bound further specifies as follows:

\[
\max\{\|U_1U_1^T - \tilde{U}_1\tilde{U}_1^T\|_F, \|V_1V_1^T - \tilde{V}_1\tilde{V}_1^T\|_F\} \leq \frac{\sqrt{2}}{\alpha} \|B - \tilde{B}\|_F,
\]

### 6.3 Spectral estimates and sums of random semidefinite matrices

The value of \(\sigma_m(X^T)\) can be estimated by certain matrix Chernoff bounds. The following theorem generalizes Hoeffding’s inequality to sums of random semidefinite matrices and was recently presented by Tropp in [63, Corollary 5.2 and Remark 5.3], improving over results in [1], and using techniques from [53] and [49].

**Theorem 6.7 (Matrix Chernoff).** Let \(X_1, \ldots, X_n\) be independent random, positive-semidefinite matrices of dimension \(m \times m\). Moreover suppose that \(\sigma_1(X_j) \leq C\) almost surely for all \(j = 1, \ldots, n\). Let

\[
\mu_{\min} = \sigma_m\left(\sum_{j=1}^n E X_j\right)
\]

be the smallest singular value of the sum of the expectations. Then

\[
P\left\{\sigma_m\left(\sum_{j=1}^n X_j\right) - \mu_{\min} \leq -s\mu_{\min}\right\} \leq m \exp\left(-\frac{\mu_{\min} s^2}{2C}\right),
\]

for all \(s \in (0, 1)\).

Recall that for some \(d_1 \times d_2\)-matrix \(A\) its spectral norm is defined as \(\max(\|AA^T\|, \|A^T A\|)^{1/2}\) (i.e. its largest singular value). For \(d_1 \times 1\)-matrices (i.e. vectors) this gives simply its \(\ell_2\)-norm.

**Corollary 6.8.** Let \(X_1, \ldots, X_N\) be independent, mean-zero \(d_1 \times d_2\)-random matrices. Assume that

\[
\|X_j\| \leq K
\]

almost surely for all \(1 \leq j \leq N\), and denote

\[
\sigma^2 = \max\left(\left\|\sum_{j=1}^N E(X_jX_j^T)\right\|, \left\|\sum_{j=1}^N E(X_j^T X_j)\right\|\right).
\]

Then it holds

\[
P\left(\left\|\sum_{j=1}^N X_j\right\| > \eta\right) \leq (d_1 + d_2) \exp\left(-\frac{\eta^2}{2(\sigma^2 + K\eta/3)}\right).
\]

We apply this result for random vectors \(Y_\ell = X_\ell - X\), where \(X = E X_\ell\), to estimate \(\|\frac{1}{N} \sum_{\ell=1}^N X_\ell - X\|\).
References


