Lower Bounds on the Generalization Error of Nonlinear Learning Models

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Abstract

We study in this paper lower bounds for the generalization error of models derived from multi-layer neural networks, in the regime where the size of the layers is commensurate with the number of samples in the training data. We derive explicit generalization lower bounds for general biased estimators, in the cases of two-layered networks. For linear activation function, the bound is asymptotically tight. In the nonlinear case, we provide a comparison of our bounds with an empirical study of the stochastic gradient descent algorithm. In addition, we derive bounds for unbiased estimators, which show that the latter have unacceptable performance for truly nonlinear networks. The analysis uses elements from the theory of large random matrices.

1 Introduction

The empirical success of deep learning is notable in a vast array of applications such as image recognition [27], speech recognition [23] and other applications [21][44]. In spite of many recent advances, this empirical success continues to outpace the development of a concrete theoretical understanding of the optimization process; in particular, the answer to the question of how and when deep learning algorithms generalize well is still open. One of the difficulties stems from the nonlinear and complex structure of these networks which are highly non-convex functions, often with millions of parameters.

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Moreover, the design of such networks for specific applications is currently mainly done in practice by trial and error.

In this paper, we derive Cramér-Rao (CR) type lower bounds \([42, 10]\) on the generalization error of these networks, when the training data is noisy. These bounds may provide insights in the process of designing and evaluating learning algorithms. Our analysis is motivated by the use of CR bounds in engineering as a benchmark for performance evaluations, see e.g. \([47, 15]\) and references therein, and as a guideline in the process of improving the experimental design. To calculate the CR bounds we combine tools from statistical estimation theory and random matrix theory. Our analysis is flexible and can be generalized to other learning tasks and architectures.

Our main findings are as follows. We provide lower bounds for general estimators, and evaluate them using random matrix theory for linear models and for feed-forward neural networks. We show that the bounds are tight for two layers neural network with linear activation function. As a comparison, we provide also a lower bound on the generalization error for unbiased estimators in nonlinear models, based on the classical CR bound; that bound is the ratio of expected \(\text{rank}\) of the Fisher information matrix to the number of samples, times the variance of the noise. We show that the expected rank of the Fisher information matrix in high dimension is large, for standard nonlinear network architectures, thereby confirming that successful learning algorithms for nonlinear networks in high dimension need to be biased.

1.1 Related literature

The connection between random matrix theory and deep learning is not new. It first appeared in the study of neural networks at initialization, for deterministic \([30, 17]\) and random \([40, 8]\) data. In these works, the matrix of interest is the conjugated kernel, i.e., the output of the last hidden layer at different data points transposed with itself. The spectrum of this kernel can then be used in the evaluation of the training error, as well as of the generalization error in the random features model in which only the last layer weights are learned \([30, 40, 8, 33]\). Random matrix theory is also used in the context of kernel learning. It is shown in \([24]\) that in the limit of large number of parameters and finite training samples, deep networks can be viewed as a kernel learning problem. Here, one of the matrices of interest is the Neural Tangent Kernel \([24]\), whose spectrum in the “linear width limit” when the number of samples is proportional to the hidden layers or features
Another matrix of interest is the Fisher information matrix which measures the amount of information about unknown parameters of the true model distribution that the training samples carry. This matrix appears in the natural gradient algorithm, since the latter is the steepest descent algorithm induced by the Fisher geometry metric. This algorithm has the advantage of being invariant under re-parametrization [2]. The Fisher matrix is also used to define a notion of complexity using the Fisher-Rao norm, en route to providing an upper bound on the generalization error of deep network with the Relu activation function [29]. The spectrum of the Fisher information matrix at initialization for one hidden layer is calculated in [41]. The Fisher matrix for deep neural network in the mean field limit is studied in [26].

There are several existing generalization upper bounds. Most of these bounds aim to estimate the capacity of the model by offering new measures of complexity excluding knowledge about the true prior of the model’s parameters. This idea is used in order to bound the generalization error from above, examples for such bounds are the PAC-Bayes bounds [32, 39, 13], VC dimension [19] parameters norms [29, 3, 38]. For the empirical evaluation of some of these generalization bounds see [25]. These approaches suggest that modern network architectures have very large capacity. Recently, lower bounds on the generalization error of linear regression models in the over-parametrized regime are derived in [4, 11, 22, 12] for specific estimators and for any interpolating estimator in [36].

1.2 Organization

The remainder of this paper is organized as follows. In Sec. 2, we present the model and assumptions. In Sec. 3, we present our main analytical results. In Sec. 4, we compare our bounds to some known estimators. In Sec. 5, we provide the proof of the main theorems. For the reader’s convenience, a review of the CR bounds is provided in Appendix A.

1.3 Notation

Throughout, boldface lowercase letters denote (column) vectors. $x^T$ denotes the transpose of a vector $x$. Uppercase letters denote matrices. For two vectors $v, w$ of the same length, $v \circ w$ denotes the vector whose $i$th entry
is $v_i \cdot w_i$. For reals $a, b$, we write $a \wedge b = \min(a, b)$. We denote by $\otimes$ the Kronecker product.

For a random vector $\theta$, the statement $\theta \sim p(\theta)$ means that $\theta$ is distributed according to the law $p(\theta)$. When a law has density with respect to Lebesgue measure on Euclidean space, we continue to use $p$ for the density; no confusion should arise from this.

We use the standard $O$ notation. Thus, sequences $a = a(d)$ and $b = b(d)$ satisfy $a = O(b)$ if there exists a constant $C$ so that $a(d) \leq Cb(d)$ for all $d$. Similarly, $a = o(b)$ if $\lim_{d \to \infty} |a/b| = 0$.

We write $\mathbb{E}$ for expectation. When we want to emphasize over which variables expectation is taken, we often write e.g. $\mathbb{E}_{x,y}$. When a conditional law is involved, we write e.g. $\mathbb{E}_{x,y/\theta}$. Thus, in the last expression, the expectation is taken with respect to the law $p(x, y/\theta)$.

For an $N \times N$ matrix $A$ with eigenvalues $\lambda_i$, we use $\rho_A = N^{-1} \sum_{i=1}^{N} \delta_{\lambda_i}$ to denote the empirical measure of eigenvalues of $A$. We use $\rho_\gamma$ to denote the Marchenko–Pastur distribution with parameter $\gamma \in (0, \infty)$, i.e., with $\lambda_\pm = (1 \pm \sqrt{\gamma})^2$,

$$d\rho_\gamma(s) = 1_{s \in [\lambda_- \lambda_+]} \sqrt{(\lambda_+ - s)(s - \lambda_-)/(2\pi \gamma s)} ds + (1 - \gamma^{-1})_+ \delta_0(s). \quad (1)$$

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## 2 Model and problem statement

We begin by setting a general framework for learning problems. We then specialize it to the feed-forward networks that are studied in this paper.

### 2.1 A general learning model

We are given a set of $M$ training samples $\{z^{(i)}\}_{i=1}^M$, such that $z^{(i)} = (x^{(i)}, y^{(i)}) \in \mathbb{R}^d \times \mathbb{R}$ are independently drawn from a distribution $p(z^{(i)}|\theta)$, parameterized by a vector $\theta \in \mathbb{R}^P$. The parameters $\theta$ are assumed random, such that $\theta \sim p(\theta)$, with $p(\theta)$ the prior distribution. We write $X \in \mathbb{R}^{d \times M}$ for the
matrix whose columns are \( x^{(i)}, y \in \mathbb{R}^M \) for the vector whose entries are \( y^{(i)} \), and set \( Z = \left( X \ y^T \right) \in \mathbb{R}^{(d+1) \times M} \).

We specialize the model to the situation where

\[
y^{(i)} = f_{\theta}(x^{(i)}) + \epsilon^{(i)}
\]

where \( f_{\theta} : \mathbb{R}^d \to \mathbb{R} \) is some representation of the real world, \( \epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2_\epsilon) \) are iid, and \( x^{(i)} \sim p(x) \); that is, the independent training samples \( x^{(i)} \) have a distribution independent of \( \theta \), while the \( y^{(i)} \)'s do depend on \( \theta \) and observation noise \( \epsilon^{(i)} \).

The estimation task at hand is to predict the output of the network \( \tilde{y} = f_{\theta}(\tilde{x}) \) on a new sample \( \tilde{x} \sim p(x) \). Formally, we seek a (measurable) estimator \( \hat{y}(\tilde{x}, Z) \). The performance of an estimator is given in terms of a loss function \( \ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R} \), which we take to be the quadratic loss \( \ell(y, y') = (y - y')^2 \); that is we consider the generalization error (population risk) \( \mathbb{E}_{Z, \tilde{x}}[\ell(\tilde{y}; \hat{y})] \). One seeks of course to minimize the population risk, and we will derive limitations on how small a risk can one achieve.

It is worthwhile to emphasize that we do not impose any constraint on the estimator \( \hat{y} \) (except for the technical measurability condition). In particular, we do not require that \( \hat{y} = f_{\tilde{\theta}}(\tilde{x}) \) for some \( \tilde{\theta} \), where \( \tilde{\theta} \) is a measurable function of \( Z \); various learning algorithms may of course use such estimators, and our lower bounds on the mean square loss will apply to them. However, the derivation of the bounds does not postulate such a structure for the estimator.

We often make the following assumption on the structure of the data.

**Assumption 2.1.** The \( x^{(i)}, i = 1, \ldots, M, \) are iid centered Gaussian vectors with covariance matrix \( \mathbb{E} x^{(i)} (x^{(i)})^T = \sigma^2_x I_d \).

This is a standard assumption, which simplifies the calculations. We believe it can be relaxed significantly (i.i.d. entries with sub-Gaussian tails should present no difficulty), however this would involve a significant amount of technical work that we chose to avoid.

### 2.2 The feed-forward setup

A feed-forward network with \( L \) layers and parameters \( W^{(l)} \in \mathbb{R}^{N_l \times N_{l-1}}, l = 1, \ldots, L \), see Figure 1, is one where

\[
f_{\theta}(x) = \frac{1}{\sqrt{N_{L-1}} \sigma^L \sigma^{L-1}}, \quad (3)
\]
with the $q^l$s, $l = 1, \ldots, L$, defined recursively as $q^1 = \frac{W^{(1)}x}{\sqrt{d}}$ and $q^l = \frac{W^{(l)}(q^{l-1})}{\sqrt{N_{l-1}}}$ for $l \geq 2$; here, $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ is a continuous function, $\sigma(x)_i = \sigma(x_i)$, and $W^{(l)}$ are the weights of the network. Since our output is a scalar, we always have $N_L = 1$. The vector $\theta \in \mathbb{R}^P$ is then taken as the collection of weights $W^{(i)}$, $i = 1, \ldots, L$, with $P = \sum_{l=1}^L N_l N_{l-1}$.

\begin{figure}[h]
\centering
\includegraphics[width=0.6\textwidth]{network_diagram.png}
\caption{Feed-forward network architecture, with $L = 4$.}
\end{figure}

We often make the following assumption on the structure of feed-forward networks.

**Assumption 2.2.** $W_{ij}^{(l)} \sim \mathcal{N}(0, \alpha_l^{-1})$, independent, with $\alpha_l > 0$, $\alpha_l = \alpha$ for $1 \leq l < L$.

Assumption 2.2 relates to the prior distribution of the weights, and probably could be relaxed to allow for more general smooth distributions; here again, using non-Gaussian weights would increase the complexity of the computations, because the Hessian of the (log of the) prior will not be deterministic.

Our last assumption is a technical assumption that allows for the use of calculus in the derivation of our bounds. It can be relaxed as in e.g., \cite{34}. We note that Assumption 2.3 is satisfied by all commonly-used activation functions, including the ReLU and sigmoid functions.

**Assumption 2.3.** The activation function $\sigma$ is five times differentiable and bounded, together with its derivatives, by some constant $K_\sigma < \infty$. 

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For convenience, we introduce the constants
\[
\eta_0(v) = \mathbb{E} \left[ \sigma^2(vz) \right] - \mathbb{E} \left[ \sigma(vz) \right]^2, \quad \xi(v) = (v \mathbb{E} \left[ \sigma'(vz) \right])^2, \\
\eta_1(v) = v^2 \mathbb{E} \left[ \sigma'(vz)^2 \right],
\]
where we recall that \( z \sim \mathcal{N}(0, 1) \), and \( v = \sigma_x / \sqrt{\alpha} \). During our analysis we will sometime use for brevity \( \xi(v) = \xi \), and \( \eta_0(v) = \eta_0 \).

### 3 Main results

As discussed in the introduction, we provide lower bounds on the generalization error of general estimator for feed-forward networks. For completeness, we also show a bound for unbiased estimators for the general learning model of Section 2.1. Our bounds are based on both Bayesian and non-Bayesian versions of the CR bound; we review the background in Appendix A. The following is our main result.

**Theorem 3.1.** Consider the model in (2), (3) with \( L = 2 \), and let Assumptions 2.1, 2.2 and 2.3 hold. Let \( \hat{y}(\tilde{x}, Z) \) be an arbitrary measurable and square integrable estimator. Then, in the regime \( M, N_1, d \to \infty \) such that \( \beta_1 = \lim_{d \to \infty} N_1 / d \in (0, \infty) \) and \( \gamma_0 = \lim_{d \to \infty} d / M \in (0, \infty) \), it holds that
\[
\mathbb{E} (\tilde{y} - \hat{y})^2 \geq \max \left( B^{(1)}, B^{(2)} \right),
\]
where
\[
B^{(1)} = \sigma_\varepsilon^2 \xi \int \frac{1 + \xi (1 - \gamma_0^{-1}) s / (\sigma^2_\varepsilon \alpha_2)}{\xi s + \alpha_2 \sigma_\varepsilon^2} d\rho_{\gamma_0^{-1}}(s) + o(1),
\]
and with \( a_1 = m_1(\sigma_\varepsilon \sqrt{\alpha_2 \beta_1}) \), and \( a_2 = m_2(\sigma_\varepsilon \sqrt{\alpha_2 \beta_1}) \),
\[
B^{(2)} = \frac{\sigma_\varepsilon}{\sqrt{\alpha_2 \beta_1}} a_1 \left( \frac{\xi}{1 + \xi a_1 a_2} + \eta_0 - \xi \right) + o(1).
\]
Here, the functions \( m_1 = m_1(u), m_2 = m_2(u) : \mathbb{C}_+ \to \mathbb{C}_+ \), satisfy for \( \Re(u) > 0 \):
\[
m_1 = \beta_1 \left( u + (\eta_0 - \xi) m_2 + \frac{\xi m_2}{\xi m_1 m_2 + 1} \right)^{-1},
\]
\[
m_2 = \frac{1}{\gamma_0} \left( u + (\eta_0 - \xi) m_1 + \frac{\xi m_1}{\xi m_1 m_2 + 1} \right)^{-1}.
\]
We note that the fixed point equations for $m_1, m_2$ have a unique solution, see in [34, Lemma 10.2] in the domain relevant for the lower bound.

The proof of Theorem 3.1 is presented in Section 5.1. We provide here several amplifying remarks.

**Remark 3.2.** It is instructive to consider several limiting cases in Theorem 3.1. In the high SNR limit, that is $\sigma_\varepsilon \to 0$, the parameter $\gamma_0$ plays a crucial role: in the underparametrized regime $\gamma_0 < 1$, as expected we get that $B^{(1)}, B^{(2)} \to \sigma_\varepsilon \to 0$. On the other hand, in the overparametrized regime $\gamma_0 > 1$, we find that $B^{(1)} \to \sigma_\varepsilon \to 0 \xi(1 - \gamma_0^{-1})/\alpha_2 > 0$, while still $B^{(2)} \to \sigma_\varepsilon \to 0$. In the low SNR limit $\sigma_\varepsilon \to \infty$, both $B^{(1)}$ and $B^{(2)}$ converge to non-zero limits (equal to $\xi/\alpha_2$ and $\eta_0/\alpha_2$, respectively). By remark 3.3, it follows that in that limit, $B^{(2)}$ is a better bound.

**Remark 3.3.** The Cauchy-Schwarz inequality together with a Gaussian integration by parts show that as soon as $\sigma$ is nonlinear, one has that $\xi = v^2(\E[\sigma'(vz)])^2 = (\E[z\sigma(vz)])^2 \leq \E[\sigma(vz)^2] = \eta_0$, and since $m_1(u), m_2(u)$ are positive, we have that $B^{(2)} > 0$.

**Remark 3.4.** The bound $B^{(1)}$ does not depend on the size of the hidden layer, as long as it is of the order of the first hidden layer, see Figure 4. This shows that in this regime one cannot recover the matrix $W^{(1)}$ with asymptotically vanishing error.

**Remark 3.5.** By construction, the bound $B^{(2)}$ is also a bound on a general estimator of the random features model in which only the weights of the last layer are being learned.

**Remark 3.6.** This theorem can be generalized to data generated by a multi-layer neural network, which represents a larger class of functions under the Gaussian assumption on the weights. This can be done by using Corollary A.6 which presents the general expression for the bound in the multi-layer case.

**Remark 3.7.** To put our result in perspective, we note that there are several generalization upper bounds for neural networks with ReLU activation function. The VC dimension for such neural networks provides essentially parameter counts, i.e. $O(LN/\sqrt{M})$ where $L$ is the number of layers, $N$ is the number of hidden units in each layers, and $M$ is the number of samples [1]. These results are improved in [3], where the factor $N$ is replaced by several norms of the layer weights. There are further results, derived using
the PAC-Bayesian framework for ReLU activation, see [39, 13]. These an-
alyze generalization behavior in neural networks, and analytically derive a
margin-based bound in terms of norms of the weights, or calculate the entire
bound empirically given the data. In our setup, to be useful all these esti-
mates require that $M \gg N^2$. In contrast, we provide analytical expression
for lower bounds on the generalization error. These bounds are on the MSE
loss for general activation function, and in the regime $M \sim N$. We note that
we allow for general estimators, while introducing special assumption on the
structure of the data, such as a Gaussianity assumption and the existence of
additive noise in the training samples.

3.1 Special cases

3.1.1 Linear activation

For linear activation, it is a straight forward to show that the optimal esti-
mator in the MMSE sense takes the following form:

$$
\hat{y}_{opt} = \frac{1}{\alpha \alpha_2 d} Y^T \left( \frac{1}{\alpha \alpha_2 d} X^T X + I_M \sigma^2 \right)^{-1} X^T \tilde{x} \tag{9}
$$

The minimum mean square error is then:

$$
\text{MMSE} = \mathbb{E} (\hat{y}_{opt} - \tilde{y})^2 = \sigma^2 \mathbb{E} \left( \frac{1}{v^2 s (1 - 1/\gamma_0) / (\sigma^2 \alpha_2) + 1} d \rho_{\gamma_0}^{-1} \right) = B^{(1)}. \tag{10}
$$

Therefore, the bound is tight in this case.

3.1.2 Highly over-parameterized regime

We explore two extreme cases:

**Finite samples size** In this regime $\beta_1 = \lim_{d \to \infty} N_1/d \in (0, \infty)$ and $M$
finite i.e. $\gamma_0 \to \infty$. Applying Theorem 3.1 with $\gamma_0 \to \infty$ we obtain $B^{(1)} = \xi/\alpha_2$, and $B^{(2)} = \eta_0/\alpha_2$. By Remark 3.3, $\eta_0 > \xi$, therefore, the bound takes the following form:

$$
\mathbb{E} (\tilde{y} - \hat{y})^2 \geq \frac{\eta_0}{\alpha_2} \tag{11}
$$

Interestingly, this does not depend on the variance of the noise. This is also
a case for which $B^{(2)} > B^{(1)}$ for non linear activation function.
Infinite samples size and input size  In this regime, the number of neurons and input size, $N_1, d$, diverges together but $N_1$ is larger than any constant times $d$, such that $\gamma_0 = \lim_{d \to \infty} d/M \in (0, \infty)$, and $\beta_1 \to \infty$. Applying Theorem 3.1, we obtain that $B^{(2)} = \eta_0/\alpha_2 + o(1)$. Since, the bound $B^{(1)}$ does not depend on the size of the number of hidden units $N_1$ as long as it is large, we obtain the following results:

$$
E(\tilde{y} - \hat{y})^2 \geq \max\left(\frac{\eta_0}{\alpha_2}, \sigma_x^2\xi \int 1 + \xi(1 - \gamma_0^{-1})s/(\sigma_x^2\alpha_2) \xi s + \alpha_2\sigma_x^2 d\rho_{\gamma_0^{-1}}(s)\right) + o(1),
$$

(12)

Note that in general whether or not $B^{(1)} > B^{(2)}$ in Theorem 3.1 depends on the activation function and the model parameters. Interestingly, in the regime of high SNR and overparametrization (see Remark 3.2), $B^{(1)}$ tends to be better, this is also observed in Figure. 2 In Figures 2, 3, and 4 below we compare the bounds for different Signal to Noise Ratio (SNR), with $SNR := 10 \log_{10}(\sigma_x^2/(\alpha_2\sigma_x^2))$, different $\gamma_0$, and different $\beta_1$. The definition of the SNR is with respect to the total variance of a linear model, $f_\theta(x) = \frac{1}{\sqrt{dN_1}}(w^{(2)})^TW^{(1)}x$, divided by the noise. The comparison is presented for four activation functions, Linear: $\sigma(x) = x$, Sigmoid: $\sigma(x) = 1/(1 + e^{-x})$, Tanh: $\sigma(x) = \tanh(x)$, and Relu: $\sigma(x) = \max(x, 0)$. That there is no clear “winner” is consistent with the analysis in [9], in which the authors consider similar types of bounds not in the context of neural networks. They compare the bounds in cases where some of the parameters are being conditioned and show via toy examples that predicting which bound is better depends on the specifics of the problem.

![Figure 2: Comparison of the bounds in Theorem 3.1 for 4 activation functions: Relu, Sigmoid, Tanh, and Linear, as function of SNR. Here, $N_1 = M = 50$, $d = 50$, $\alpha = 1$, $\alpha_2 = 2$, and $\sigma_x^2 = 1$. The dashed blue line is (7). The solid red line is (8).](image-url)
Figure 3: Comparison of the bounds in 3.1 as function of $\gamma_0$. Here, $N_1 = 100$, $d = 100$, $\alpha = \alpha_2 = 1$, $\sigma^2_x = 0.1$ and $\sigma^2_x = 1$. The dashed blue line is (7). The solid red line is (8).

Figure 4: Comparison of the bounds in Theorem 3.1 as a function of the $\beta = \frac{N_1}{d}$. Here $N_1 = d = 50$, $\alpha = \alpha_2 = 1$, and $\sigma^2_x = 1$. The dashed blue line is (7). The solid red line is (8).

### 3.2 Unbiased estimators

So far we discussed the Bayesian version of the CR bound. In this subsection we provide as a comparison the classical version of the CR bound, which does not require knowledge about the prior distribution of the parameters, but makes however an unbiasedness assumption on the estimator. Recall that the bias of an estimator $\hat{y}(\tilde{x},Z)$ is $b_\theta(\tilde{x}) = f_\theta(\tilde{x}) - \mathbb{E}_{Z|\theta,\tilde{x}}\hat{y}(\tilde{x},Z)$. **Unbiased estimators** are those which satisfy $b_\theta(\tilde{x}) = 0$, almost surely. Note that the minimum mean square error (MMSE) estimator $\hat{y}_{opt} = \mathbb{E}[\hat{y}|\tilde{x}, Z]$ is typically not unbiased.

As experience shows, in high dimension biased estimators can significantly outperform biased ones. Theorem [3.8] whose proof is provided in Section 5.2 together with Theorem [B.2] in the appendix, show that indeed unbiased estimators have bad performance in the truly nonlinear setup; see Remark [B.4].

The CR bound for unbiased estimators involves the Fisher information
\( I(\theta) \in \mathbb{R}^{P \times P} \), which in our case takes the form

\[
I(\theta) = \frac{M}{\sigma_\varepsilon^2} A(\theta), \quad A(\theta) = \mathbb{E}_x \left[ \nabla_{\theta} f_\theta(x) \nabla_{\theta} f_\theta(x)^T \right]. \tag{13}
\]

**Theorem 3.8.** Consider the model in (2). Assume that \( \nabla_{\theta} f_\theta(x) \) exists and is square integrable under \( p(x) \). Let \( \hat{y}(x, Z) \) be any square integrable unbiased estimator. Then,

\[
\mathbb{E}_{Z, \tilde{x}|\theta} \left[ (\hat{y} - \hat{y})^2 \right] \geq \sigma_\varepsilon^2 \frac{\text{Rank}(I(\theta))}{M}. \tag{14}
\]

The proof of Theorem 3.8 is provided in Section 5.2. In Appendix B we evaluate the rank of the Fisher information in a few examples. We show that the reason for high rank (and then bad performance) is a combination of high dimension phenomena with the non-linearity of the model.

## 4 Performance evaluation

In this section, we compare the bounds of Theorem 3.1 to the performance of estimators used in practice. Since an analytic expression for the optimal estimator is not known, we instead compare numerically the bounds to the performance of an estimator based on the stochastic gradient descent algorithm \[43\], which is one of the most common algorithm used to train neural network models. We do so in the framework of the “teacher-student model” \[45, 16\], which we describe next.

### 4.1 Data generation (teacher network)

Following the “teacher-student model”, we generate numerically \( N_\theta \) realization of the teacher true weights \( \theta = (w^{(2)}; W^{(1)}) \) of a two layers neural network. The weights vector \( \theta \) is drawn from a Gaussian distribution with zero mean and variance \( \alpha = 1 \) for each element in the matrix \( W^{(1)} \), and variance \( \alpha_2 = 1 \) for each element of the vector \( w^{(2)} \). For each true realization of \( \theta \), we generate \( N_d \) data-sets of size \( M \), and a test set of size \( N_s \). Each training sample \( x^{(i)} \sim \mathcal{N}(0, \sigma_x^2 I_d) \), and \( y^{(i)} = (w^{(2)})^T \sigma(W^{(1)} x^{(i)}/\sqrt{d})/\sqrt{N_1} + \varepsilon^{(i)} \), where \( \varepsilon^{(i)} \sim \mathcal{N}(0, \sigma_\varepsilon^2) \).
4.2 Estimator (student network)

Given the data generated by the teacher network, we use a two layers neural
network with twice as large number of neurons in the hidden layer then the
teacher network. The estimator is obtained by running a stochastic gradient
descent (SGD) algorithm \[43\] for \( N_{\text{epochs}} = 100 \) epochs and batch size \( N_b = 5 \)
with learning rate \( \eta = 0.5/M \) for Sigmoid and \( \eta = 0.01/M \) for Tanh, linear
and Relu. The generalization error is obtained by averaging over all these
quantities.

Figure 5 presents the results for two variances \( \sigma^2 \) of the noise. In Figure 6,
the bounds are compared to the performance of SGD with data generated by
a teacher network with the same size as before but with uniform prior on the
weights in both layers. The variance of the weights matches the variance in
the Gaussian case. In this case, even though the weights are not drawn form
a Gaussian prior, the numerical results suggest that the bounds do apply. In
both figures we also compare the performance of SGD to the performance of
a trivial mean predictor, \( \bar{y}_{\text{mean}} = \sum_{i=1}^{M} y_i/M \).

5 Proof of the main Theorems

We recall elements of the Cramér-Rao theory in Appendix A.

5.1 Proof of Theorem 3.1

We will use Corollary [A.6] for depth \( L = 2 \), which states that

\[
E_g \geq \max(B^{(1)}, B^{(2)})
\]

Recall that following \[3\] for \( L = 2 \) and \( N_1 = N \), \( f_\theta(x) = (w^{(2)})^T \sigma(q)/\sqrt{N} \),
and \( q = W^{(1)}x/\sqrt{d} \). The gradient is then

\[
\nabla_\theta f_\theta(x) = \begin{bmatrix}
\nabla_{W^{(1)}} f_\theta(x) \\
\nabla_{w^{(2)}} f_\theta(x)
\end{bmatrix} = \begin{bmatrix}
\frac{1}{\sqrt{Nd}} D^{1} w^{(2)} \otimes x \\
\frac{1}{\sqrt{N}} \sigma(q)
\end{bmatrix},
\]

where \( D^{1} = \text{diag}(\sigma'(q)) \). In the following, we evaluate separately \( B^{(1)} \) and
\( B^{(2)} \).
Figure 5: The generalization performance of SGD and the bounds in Theorem 3.1 as function of $\gamma_0 = d/M$. The generalization error of SGD is in black dots, and its bias in green dots. The performance of trivial mean predictor are in magenta. The dashed blue line is the bound (7), while the red solid line is (8). In the top panel, $\sigma^2_e = 0.02$ and in the bottom panel, $\sigma^2_e = 0.2$. Other parameters are $N_1 = d = 50, \alpha = \alpha_2 = \sigma^2_x = 1$.

Evaluation of $B^{(1)}$: Take $\theta_l = w^{(2)}$ in Corollary A.6. Then, the bound in (72) reads

$$B^{(1)} = \frac{\sigma^2_e}{d} \mathbb{E}_{w^{(2)}, X} \left[ \text{Tr} \left( (I(X, w^{(2)}) + \sigma^2_e \alpha I_N)^{-1} Q(w^{(2)}) \right) \right],$$

(16)

where

$$Q(w^{(2)}) = d\mathbb{E}_{\tilde{x}} \left[ \mathbb{E}_{W^{(1)}} \nabla_{W^{(1)}} f_{\theta}(\tilde{x}) \left( \mathbb{E}_{W^{(1)}} \nabla_{W^{(1)}} f_{\theta}(\tilde{x}) \right)^T \right]$$

$$= \frac{1}{N} \mathbb{E}_{\tilde{x}} \left[ \tilde{D}^1 w^{(2)}(w^{(2)})^T \tilde{D}^1 \otimes \tilde{x}\tilde{x}^T \right],$$

(17)
Figure 6: The generalization performance of SGD vs the bounds in Theorem 3.1 as function of $\gamma_0 = d/M$. The data given by the teacher is generated with a uniform prior on the weights, i.e. $W_{ij}^{(1)}, w_i^{(2)} \sim U(-b, b)$, where $b = \sqrt{3}/\alpha$. The generalization error of SGD is in black dots, and its bias in green dots. The performance of trivial mean predictor are in magenta. The dashed blue line is the bound (7), while the red solid line is (8). The parameters are $N_1 = d = 50, \alpha = \alpha_2 = \sigma_x^2 = 1$ and $\sigma_e^2 = 0.02$. The student network is with 150 hidden units.

$\bar{D}^1 = \mathbb{E}_{W^{(1)}}[D^1]$, and the Fisher matrix which appears in the bound following (18) is

\[
I(X, w^{(2)}) = \sum_{k=1}^{M} \mathbb{E}_{W^{(1)}, w^{(2)}, X} \left[ \nabla_{W^{(1)}} f_{\theta}(x^{(k)}) \nabla_{W^{(1)}} f_{\theta}(x^{(k)})^T \right] \\
= \sum_{k=1}^{M} \mathbb{E}_{W^{(1)}, w^{(2)}, X} \left[ D^{1(k)}(w^{(2)})(w^{(2)})^T D^{1(k)} \otimes x^{(k)}(x^{(k)})^T \right] \tag{18}
\]

where $q^{(k)} = W^{(1)}x^{(k)}/\sqrt{d}$ and $D^{1(k)} = \text{diag}(\sigma'(q^{(k)}))$. Our work is then to evaluate the asymptotics of the right side of (16). Toward this end, we first show that we can replace $Q(w^{(2)})$ in the latter by the simpler matrix

\[
\tilde{Q}(w^{(2)}) = \frac{\alpha \xi}{N} w^{(2)}(w^{(2)})^T \otimes I_d, \tag{19}
\]
such that the error due to this replacement goes to zero in the limit of $d \to \infty$. Indeed, the replacement error reads

$$\frac{\sigma^2}{d} \mathbb{E} \left[ \left\| \text{Tr} \left( (I(X, w^{(2)}) + \sigma^2 \alpha I_{Nd})^{-1} (Q - \tilde{Q}) \right) \right\| \right] \leq \frac{1}{\alpha d} \mathbb{E} \left[ \|Q - \tilde{Q}\|_* \right]$$

$$\leq \sqrt{\frac{N}{d}} \frac{1}{\alpha} \mathbb{E} \left[ \|Q - \tilde{Q}\|_{HS} \right] \xrightarrow{d \to \infty} 0, \quad (20)$$

where $\| \cdot \|_*$ denotes the nuclear norm, the first inequality is due to the positive definiteness of $I(X, w^{(2)})$ which implies that the operator norm of the inverse is bounded above by $1/\alpha \sigma^2$, the second follows from the Cauchy-Schwarz inequality, and the limit follows from Lemma 5.1.

Introduce the constants

$$\nu_x^{(k)} = \|x^{(k)}\|_2/\sqrt{d \alpha}, \quad \eta_1^{(k)} = \mathbb{E}_z \left[ \sigma' (z r_x^{(k)})^2 \right], \quad \xi^{(k)} = \mathbb{E}_z \left[ \sigma' (z r_x^{(k)}) \right]^2, \quad (21)$$

where $z \sim \mathcal{N}(0, 1)$. We next show that we can also replace the matrix $I(X, w^{(2)})$ by the matrix $\tilde{I}(X, w^{(2)})$, where

$$\tilde{I}(X, w^{(2)}) = \frac{\xi}{\nu^2 N d} w^{(2)} (w^{(2)})^T \otimes XX^T + G(X, w^{(2)}) =: \tilde{I}(X, w^{(2)}) + G(X, w^{(2))},$$

with

$$G(X, w^{(2)}) = \frac{1}{N} \sum_k D^{(2)} \otimes \frac{1}{d} c^{(k)} (x^{(k)})^T,$$  

$$D^{(2)}_{ij} = \delta_{ij} \left( w_i^{(2)} \right)^2 \quad \text{and} \quad c^{(k)} = \eta_1^{(k)} - \xi^{(k)}. \quad (22)$$

Set $I_\alpha = I(X, w^{(2)}) + \sigma^2 \alpha I_{Nd}$ and $\tilde{I}_\alpha = \tilde{I}(X, w^{(2)}) + \sigma^2 \alpha I_{Nd}$. The error due to the replacement of $I$ by $\tilde{I}$ is then

$$\frac{1}{\alpha^2 d} \mathbb{E} \left[ \text{Tr} \left( \left( I_\alpha^{-1} - \tilde{I}_\alpha^{-1} \right) Q \right) \right] \leq \frac{1}{\alpha^2 d} \mathbb{E} \left[ \text{Tr} \left( \tilde{I}_\alpha^{-1} \left( I_\alpha^{-1} - I_\alpha \right) I_\alpha^{-1} Q \right) \right]$$

$$\leq \frac{1}{\alpha^2 d} \mathbb{E} \left[ \text{Tr} \left( Q \right) \|I - \tilde{I}\|_{op} \right] \leq \frac{\xi}{\alpha} \sqrt{\mathbb{E} \left[ \|w^{(2)}\|^2 \right]} \sqrt{\mathbb{E} \left[ \|I - \tilde{I}\|^2_{op} \right]}$$

$$\leq \frac{\xi}{\alpha \sigma_2} \sqrt{\mathbb{E} \left[ \|I - \tilde{I}\|^2_{op} \right]} ; \quad (24)$$

In the first equality we used the identity

$$A^{-1} - B^{-1} = A^{-1} (B - A) B^{-1}, \quad (25)$$
in the first inequality we used the positive definiteness of $\tilde{Q}$ and that $\|\hat{I}_\alpha^{-1}\|_{op} \leq \alpha^{-1}$, in the second inequality we used the Cauchy-Schwarz inequality, and in the last Assumption 2.2. An application of Lemma 5.2 below then shows that $\mathbb{E}\left[\|I - \tilde{I}\|_{2}^2\right] \xrightarrow{d \to \infty} 0$, and completes the justification of the replacement of $I$ by $\tilde{I}$. We thus obtained that

$$B^{(1)} = \frac{\sigma_x^2}{d} \mathbb{E} \text{Tr}(\tilde{I}_\alpha^{-1} \tilde{Q}) + o(1). \quad (26)$$

We next show that we can replace $\tilde{I}_\alpha$ in (26) by $\tilde{I}_\alpha = \hat{I}_\alpha - G = \hat{I}(X, w^{(2)}) + \sigma_x^2 \alpha I_{Nd}$, i.e. remove $G$ in (22), with an $o(1)$ error. Indeed, using the identity (25) with $A = \tilde{I}_\alpha$ and $B = \hat{I}_\alpha$, and using that $\|\tilde{I}_\alpha\|_{op}, \|\hat{I}_\alpha\|_{op} \leq 1/\alpha \sigma_x^2$ we obtain, using that the rank of $\tilde{Q}$ is bounded above by $d$, that

$$\frac{1}{d} \mathbb{E} \text{Tr}((\tilde{I}_\alpha - \hat{I}_\alpha) \tilde{Q}) \leq C \mathbb{E}[\|\tilde{G}\|_{op}\|\tilde{Q}\|_{op}], \quad (27)$$

where $C$, here and in the next few lines, is a constant independent of $d$. By construction, $\mathbb{E}\|\tilde{Q}\|_{op}^2 \leq C$. Also, from standard properties of Wishart matrices, $\mathbb{E}\|d^{-1} \sum_k \mathbf{x}^{(k)}(\mathbf{x}^{(k)})^T\|_{op}^4 \leq C$ while, using that the entries $w_i^{(2)}$ are standard i.i.d. Gaussians, $\mathbb{E} \max_i(w_i^{(2)})^4 \leq C(\log d)^2$ and therefore $\mathbb{E}\|G\|_{op}^2 \leq C \log d/N^2$. Therefore, the right hand side of (27) is bounded above by $\sqrt{\log d/N} = o(1)$. Altogether, we obtain that

$$B^{(1)} = \frac{\sigma_x^2}{d} \mathbb{E} \text{Tr}(\tilde{I}_\alpha^{-1} \tilde{Q}) + o(1). \quad (28)$$

Set $J_w = w^{(2)} \otimes I_d/\sqrt{N} \in \mathbb{R}^{Nd \times d}$, and $J_{X,w} = w^{(2)} \otimes X/\sigma_x \sqrt{Nd} \in \mathbb{R}^{Nd \times M}$. Then,

$$B^{(1)} = \frac{\sigma_x^2 \alpha \xi}{d} \mathbb{E} \left[ \text{Tr} \left( \left( \alpha \xi J_{X,w} J_{X,w}^T + \alpha \sigma_x^2 I_{Nd} \right)^{-1} J_w J_w^T \right) \right] + o(1). \quad (29)$$

By Woodbury’s formula, we have that

$$(\alpha \xi J_{X,w} J_{X,w}^T + \alpha \sigma_x^2 I_{Nd})^{-1} = (\alpha \sigma_x^2)^{-1} I_{Nd}$$

$$- (\alpha \sigma_x^2)^{-2} \alpha \xi J_{X,w} (I_M + \sigma_x^{-2} \xi J_{X,w} J_{X,w})^{-1} J_{X,w}^T \quad (30)$$
Substituting (30) back in (29), we have that:

\[
B^{(1)} = o(1) + \frac{\xi}{d} E_{w(2)} \left[ \text{Tr} \left( J_{w}^{T} J_{w} \right) \right] - \frac{\xi^2}{\sigma^2 \epsilon} E_{w(2),X} \left[ \frac{1}{d} \text{Tr} \left( \left( I_M + \frac{\xi}{\sigma^2 \epsilon} J_{X,w} J_{X,w} \right)^{-1} J_{X,w}^{T} J_{w} J_{X,w}^{T} \right) \right]
\]

where we define \( r_w = \|w^{(2)}\|_2^2 / N \). The first term in the right hand side of (31) is simply

\[
\frac{1}{d} E_{w(2)} \left[ \text{Tr} \left( J_{w}^{T} J_{w} \right) \right] = \frac{1}{d} E_{w(2)} \left[ \text{Tr} \left( (w^{(2)})(w^{(2)})^T \otimes I_d \right) \right] = E_{w(2)} r_w = \frac{1}{\alpha^2}.
\] (32)

To analyze the second term, we first calculate,

\[
J_{X,w}^{T} J_{w} = \left( \frac{1}{\sqrt{Nd}} (w^{(2)})^T \otimes X^T \right) \left( \frac{1}{\sqrt{N}} w^{(2)} \otimes I_d \right) = r_w \frac{1}{\sqrt{d}} X^T
\] (33)

Hence, \( J_{X,w}^{T} J_{w} J_{X,w} = r_w^2 X^T X / d \). We also have that

\[
J_{X,w}^{T} J_{X,w} = \left( \frac{1}{\sqrt{Nd}} (w^{(2)})^T \otimes X^T \right) \left( \frac{1}{\sqrt{Nd}} w^{(2)} \otimes X \right) = r_w \frac{1}{d} X^T X
\] (34)

Using (33) and (34) the bound in the right hand side of (31) reads:

\[
\frac{\xi}{\alpha^2} - \frac{\xi^2}{\sigma^2 \epsilon} E_{w(2),X} \left[ \frac{1}{d} \text{Tr} \left( \left( I_M + \frac{\xi}{\sigma^2 \epsilon} r_w \frac{1}{d} X^T X \right)^{-1} r_w^2 \frac{1}{d} X^T X \right) \right]
= \frac{\xi}{\alpha^2} - \xi^2 E_{w(2),X} \left[ \frac{1}{d} \sum_i \frac{r_w^2 \lambda_i (\frac{1}{d} X^T X)}{\sigma^2 + \xi r_w \lambda_i (\frac{1}{d} X^T X)} \right].
\] (35)

By dominated convergence and the convergence of the empirical measure of eigenvalues of \( X^T X / d \) in the regime \( M, d \to \infty \) such that \( \gamma_0 = \lim_{d \to \infty} d/M \in (0, \infty) \) to the Marchenko-Pastur law and the convergence of \( r_w \) to \( 1/\alpha^2 \), the last expression converges (as \( d \to \infty \)) to

\[
\frac{\xi}{\alpha^2} \left( 1 - \frac{\xi}{\gamma_0} \int \frac{s}{\xi s + \alpha_2 \sigma^2 \epsilon} d\rho_{\gamma_0^{-1}}(s) \right)
= \sigma^2 \epsilon \int \frac{1 + \xi (1 - \gamma_0^{-1}) s / \sigma^2 \epsilon \alpha^2}{\xi s + \alpha_2 \sigma^2 \epsilon} d\rho_{\gamma_0^{-1}}(s).
\] (36)

This yields (7).
Evaluation of $B^{(2)}$ 

The bound $B^{(2)}$ is derived by taking $\theta_t = W^{(1)}$ in Corollary A.6. Hence, following (72), the bound reads

$$B^{(2)} = \frac{1}{N} \mathbb{E}_{W^{(1)},X} \left[ \text{Tr} \left( \left( I(X, W^{(1)}) \right)^{-1} \Sigma(W^{(1)}) \right) \right],$$

where $X \in \mathbb{R}^{d \times M}$ is the features matrix and $x^{(k)} \in \mathbb{R}^{d \times 1}$ are its columns, the matrix $\Sigma = \Sigma(W^{(1)}) \in \mathbb{R}^{N \times N}$ is

$$\Sigma(W^{(1)}) = \mathbb{E}_x \left[ \sigma(q)\sigma(q)^T \right],$$

and the Fisher matrix $I$ is

$$I(X, W^{(1)}) = \frac{1}{\sigma^2} \sum_{k=1}^{M} \sigma(q^{(k)})\sigma(q^{(k)})^T + \alpha_2 I_N,$$

where $q^{(k)} = W^{(1)}x^{(k)}/\sqrt{d}$. Substituting the matrices (38) and (39) in (37), such that $X^{(1)} = \sigma(W^{(1)}X/\sqrt{d}) \in \mathbb{R}^{N \times M}$, we obtain that

$$B^{(2)} = \frac{\sigma^2}{d} \mathbb{E}_{W^{(1)},X} \left[ \text{Tr} \left( \left( \frac{1}{d} X^{(1)}(X^{(1)})^T + \frac{1}{d} \Sigma \right)^{-1} \right) \right] = \frac{\sigma^2}{d} \mathbb{E}_{W^{(1)},X} \left[ \text{Tr} \left( \left( \frac{1}{d} X^{(1)}(X^{(1)})^T + \alpha d I_N \right)^{-1} \right) \right],$$

where we define $\alpha_d = N\sigma_e^2/\alpha_2$. To calculate the expression above, we utilize the framework in [34] adapted to our settings. We first note that by Lemma 5.3 the operator norm difference between the matrix $\Sigma$ and the matrix

$$\tilde{\Sigma} = I_N(\eta_0 - \xi) + \alpha_2 \frac{1}{d} W^{(1)}(W^{(1)})^T + \frac{a}{d} \left( 1_N 1_N^T - I_N \right)$$

(with $a \in \mathbb{R}$ an appropriate constant) is $o(1)$. The error due to this replacement is bounded by $\|\Sigma - \tilde{\Sigma}\|_{op}/\alpha_2$, hence the expected error goes to zero. Next, note that the contribution of the third term in (41) is $o(1)$ since

$$\frac{\sigma^2}{d^2} \left| \text{Tr} \left( \left( \frac{1}{d} X^{(1)}(X^{(1)})^T + \alpha_d I_N \right)^{-1} (1_N 1_N^T - I_N) \right) \right| \leq \frac{1}{\alpha_2 d}.$$ 

Therefore, to calculate (40) we need to evaluate the two terms
\[ T_1 = \mathbb{E}_{W^{(1)}, X} \left[ \frac{1}{d} \text{Tr} \left( \left( \frac{1}{d} X^{(1)} (X^{(1)})^T + \alpha_d I_N \right)^{-1} \right) \right] \]

and

\[ T_2 = \mathbb{E}_{W^{(1)}, X} \left[ \frac{1}{d} \text{Tr} \left( \left( \frac{1}{d} X^{(1)} (X^{(1)})^T + \alpha_d I_N \right)^{-1} W^{(1)} (W^{(1)})^T \right) \right]. \]

Adopting the notation of \cite{34}, we consider the following matrix \( A(s) \in \mathbb{R}^{r \times r} \), where \( r = M + N \):

\[ A(s) = \begin{bmatrix} s_1 I_N + s_2 Q & (X^{(1)})^T \\ X^{(1)} & 0_M \end{bmatrix}. \]

For our purposes, we take \( s = (s_1, s_2) \in \mathbb{R}^2 \), and \( Q_{ij} = \frac{1}{d} \sum_k W^{(1)}_{ik} W^{(1)}_{jk} \). For \( t \in \mathbb{C}_+ \), we introduce the log-determinant

\[ G_d(t, s) = \frac{1}{d} \sum_{i=1}^r \log(\lambda_i(A) - t) = \frac{1}{d} \log \left( \det (A(s) - tI_r) \right) + i2\pi k(s, t), \]

where \( k(s, t) \in \mathbb{N} \), and the Stieltjes transform of the empirical measure of eigenvalues of \( A(s) \)

\[ M_d(t, s) = \frac{1}{d} \sum_i (\lambda_i(A) - t)^{-1} = -\frac{d}{dt} G_d(t, s). \quad (42) \]

Using the definition of the log-determinant and applying simple algebraic manipulations, see \cite{34} Appendix B] for more details, we then have

\[ \partial_{s_1} G_d(iu, 0) = \frac{1}{d} \text{Tr} \left( (A(0) - iu I_r)^{-1} \partial_{s_1} A(0) \right) \]

\[ = \frac{1}{d} \text{Tr} \left( (A(0) - iu I_r)^{-1} \partial_{s_1} A(0) \right) \]

\[ = \frac{1}{d} \text{Tr} \left( (-iuI_N + (iu)^{-1} X^{(1)}(X^{(1)})^T)^{-1} \right) = iu \frac{1}{d} \text{Tr} \left( (u^2 I_N + X^{(1)}(X^{(1)})^T)^{-1} \right) \]

and

\[ \partial_{s_2} G_d(iu, 0) = \frac{1}{d} \text{Tr} \left( (A(0) - tI_r)^{-1} \partial_{s_2} A(0) \right) \]

\[ = \frac{1}{d} \text{Tr} \left\{ (-iuI_N - iu^{-1} X^{(1)}(X^{(1)})^{-1} Q \right\} \]

\[ = iu \frac{1}{d} \text{Tr} \left\{ (u^2 I_N + X^{(1)}(X^{(1)})^{-1} Q \right\}. \]
Therefore, substituting in (40),
\[
\sigma^2 \left[ \alpha \xi T_2 + (\eta_0 - \xi) T_1 \right]
= -\sigma^2 \left[ \alpha \xi \partial_z G_d(iu_c, 0) + (\eta_0 - \xi) \partial_z G_d(iu_c, 0) \right] ,
\]
where \( u_c = \sigma \sqrt{\alpha / \beta} \).

Introduce the (deterministic) functions
\[
g(t, s) = \Xi(t, z_1, z_2) |_{(z_1, z_2) = (m_1(t,s), m_2(t,s))}
\]
and
\[
\Xi(t, z_1, z_2) = \log \left[ (s_2 z_1 + 1) - \xi z_1 z_2 \right] - (\eta_0 - \xi) z_1 z_2 + s_1 z_1 - \beta_1 \log \left( \frac{z_1}{\beta_1} \right) - \frac{1}{\gamma_0} \log \left( \gamma_0 z_2 \right) - \xi (z_1 + z_2) - \beta_1 - \frac{1}{\gamma_0},
\]
where the functions \( m_1(\cdot; s), m_2(\cdot; s) : \mathbb{C}_+ \rightarrow \mathbb{C}_+ \) are the unique analytic solutions in \( \mathbb{C}_+ \) with growth \( 1/\xi \) at infinity, of the following equations:
\[
m_1 = \beta_1 \left( -t + s_1 - (\eta_0 - \xi) m_2 + \frac{s_2 - \xi m_2}{1 + s_2 m_1 - \xi m_1 m_2} \right)^{-1}
\]
\[
m_2 = \frac{1}{\gamma_0} \left( -t - (\eta_0 - \xi) m_1 - \frac{s_1 - \xi m_1}{1 + s_2 m_1 - \xi m_1 m_2} \right)^{-1},
\]
where we wrote for brevity \( m_1 = m_1(t; s) \) and \( m_2 = m_2(t; s) \). (That the solutions of (44) and (45) are unique and analytic in a neighborhood of \( \infty \) follows from the implicit function theorem, and the uniqueness in \( \mathbb{C}_+ \) follows from analytic continuation.) By [34, Proposition 8.4], we have that for any fixed \( t \in \mathbb{C}_+ \),
\[
\mathbb{E} \left[ G_d(t, s) - g(t, s) \right] + \mathbb{E} \left\| \nabla_s G_d(t, 0) - \nabla_s g(t, 0) \right\|^2 \rightarrow_{d \to \infty} 0.
\]
(We remark that by [34, Proposition 8.3], the Stieltjes transform \( M_d(t, s) \) of (42) converges uniformly in compacts, in probability, to \( m_1 + m_2 \) as in (44) and (45).)

Summarizing, we have that
\[
B^{(2)} = -\sigma^2 \left[ \alpha \xi \partial_z G_d(iu_c, 0) + (\eta_0 - \xi) \partial_z G_d(iu_c, 0) \right] + o(1),
\]
so that it only remains to evaluate the derivatives of \( g \) appearing in (47). Toward this end, we note, following [34], that the fixed point equations (44) and (45) imply that \((m_1; m_2)\) is a stationary point of the function \( \Xi(t, \cdot, \cdot, s) \), that is \( \partial_{z_i} \Xi(t, z_1, z_2, (s))|_{z_1=m_1, z_2=m_2} = 0 \) for \( i = 1, 2 \). This simplifies the calculation of derivatives with respect to \( s \) and yields, by taking the derivative of \( \Xi \) with respect to \( s \), that

\[
\partial_s g(t, 0) = \frac{m_1}{1 - \xi m_1 m_2},
\]

and

\[
\partial_{s_i} g(t, 0) = m_i.
\]

Specializing (44) and (45) to \( s = 0 \) and using, with a slight abuse of notation, \( m_i = m_i(t, 0) \), we have thus obtained that

\[
m_1 = \beta_1 \left( -t - (\eta_0 - \xi) m_2 + \frac{\xi m_2}{\xi m_1 m_2 - 1} \right)^{-1}
\]

and

\[
m_2 = \frac{1}{\gamma_0} \left( -t - (\eta_0 - \xi) m_1 + \frac{\xi m_1}{\xi m_1 m_2 - 1} \right)^{-1}.
\]

and, from (47) with \( t_c = i u_c, \)

\[
B^{(2)} = -\frac{\sigma_s}{\sqrt{\alpha_2 \beta_1}} im_1(t_c) \left[ \frac{\xi}{1 - \xi m_1(t_c) m_2(t_c)} + \eta_0 - \xi \right] + o(1).
\] (48)

Note that, by definition, for \( t = ib \) when \( b > 0 \), \( m_1(ib) \) and \( m_2(ib) \) are purely imaginary and \( \Im m_1(ib) \); \( \Im m_2(ib) > 0 \), hence the expression in (48) is real valued. The theorem is obtained by making the substitutions \( m_i \rightarrow -im_i. \)

We now provide the proof of lemmas used above. Recall the definition of the matrices \( Q \) and \( \tilde{Q} \), see (17) and (19).

**Lemma 5.1.** Let Assumptions 2.1, 2.2 and 2.3 hold. Then, in the regime \( N, d \rightarrow \infty \) such that \( \beta_1 = \lim_{d \rightarrow \infty} N/d \), it holds that \( \mathbb{E} \left[ \| Q - \tilde{Q} \|_{HS} \right] \rightarrow 0 \)

**Proof.** Recall the definition of the matrix

\[
Q = \frac{1}{N} \mathbb{E}_{\tilde{x}} \left[ \tilde{D}^1 w^{(2)}(w^{(2)})^T \tilde{D}^1 \otimes \tilde{x} \tilde{x}^T \right],
\] (49)
where \( \bar{D} = E_{W(1)}[\text{diag}(\sigma'(q_{wi}))] \), and \( q_{wi} = W^{(1)}x/\sqrt{d} \). Typical elements in the matrix \( \bar{Q} \) are of the form

\[
Q_{i_1,i_2,i'_2,i'_3} = \frac{1}{N} w_{i_1}^{(2)} w_{i_2}^{(2)} E_x [E_{W(1)} \sigma'(q_{wi_2}) E_{W(1)} \sigma'(q_{wi_3}) x_{i'_2} x_{i'_3}] \tag{50}
\]

Since by assumption \( W^{(1)} \) is a Gaussian matrix, the variables \( q_{wi} \sim \mathcal{N}(0, r_x^2) \) for all \( i \), where \( r_x = \|x\|_2/\sqrt{\alpha d} \). Therefore, \( E_{W(1)}[\sigma'(q_{wi})] = E_z[\sigma'(z r_x)] \), with \( z \sim \mathcal{N}(0,1) \). Write for brevity \( g(\|x\|^2/d) = E_z[\sigma'(z r_x)]^2 \) and \( \tilde{z}_{i,i'_1} = \sum_{k \neq i_1,i'_1} x_k^2/d \). Applying a Taylor expansion around \( \tilde{z}_x \), we obtain

\[
E \left[ x_{i'_1} x_{i_1} g \left( \frac{\|x\|^2}{d} \right) \right] = \delta_{i_1 i'_1} \sigma_x^2 E[g(\tilde{z}_{i_i,i'_1})] + \delta_{i_1 i'_1} \frac{1}{d} \frac{6 \sigma_x^4}{2} E\left[ g(\tilde{z}_{i_i,i'_1}) \right] + \frac{1}{d^2} E_{i_1 i'_1} \tag{51}
\]

where \( E_{i_1 i'_1} = E \left[ x_{i'_1} x_{i_1} (x_{i'_1}^2 + x_{i_1}^2) \right] /2 \) and \( \eta_{i,i'_1} \) is a random point between \( \tilde{z}_{i,i'_1} \) and \( \|x\|^2/d \). Using Chebyshev’s inequality, \( \|x\|^2/d \to \sigma_x^2 \) in probability, and since by assumption \( \sigma' \) is bounded, the bounded convergence theorem yields that \( E[g(\tilde{z}_{i_i,i'_1})] \to \alpha \xi \). Since \( g' \) is bounded by assumption, \( E\left[ g(\tilde{z}_{i_i,i'_1}) \right] \) is also some bounded constant which do not depend on the index \( i_1 \). Therefore, substituting back in (50), the first term yields the matrix \( \bar{Q} \).

We now calculate the error \( E \left[ \|Q - \bar{Q}\|_{\text{HS}} \right] \) due to the second and third terms in (51). The error from the second term is \( o(1) \) since

\[
\frac{1}{dN} E \left[ \|I_d \otimes w^{(2)}(w^{(2)})^T\|_{\text{HS}} \right] = \frac{1}{\sqrt{dN}} E \left[ \|w^{(2)}(w^{(2)})^T\|_{\text{HS}} \right] \leq \frac{1}{\sqrt{d\alpha_2}}. \tag{52}
\]

The error due to the third term is also \( o(1) \) since

\[
\frac{1}{d^2 N} E \left[ \|w^{(2)}(w^{(2)})^T\|_{\text{HS}} \right] \|E\|_{\text{HS}} \leq \frac{\|E\|_{\text{HS}}}{d^2} \leq \frac{c}{d}, \tag{53}
\]

since by the Cauchy-Schwarz inequality, the boundedness of \( g'' \), and the fact that \( x \) has finite moments by assumption, we have that \( \|E\|_{\text{HS}} \leq d c \) where \( c \) is a constant independent of \( d \). Therefore the error due to the forth term is \( o(1) \). This completes the proof.

Recall the constants in (21), and the matrices \( I, \bar{I} \), see (22) and (18).

**Lemma 5.2.** Let Assumptions 2.1, 2.2 and 2.3 hold. Then, in the regime 
\( N, d, M \to \infty \) such that \( r_0 = \lim_{d \to \infty} d/M \in (0, \infty) \) and \( \beta_1 = \lim_{d \to \infty} N/d \), it holds that \( E \left[ \|I - \bar{I}\|_{\text{op}}^2 \right] \to 0 \).

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Proof. Write
\[ I(X, w^{(2)}) = \sum_k \mathbb{E}_{W^{(1)}|w^{(2)}, X} \left[ s_w^{(k)} (s_w^{(k)})^T \otimes \frac{1}{d} x^{(k)} (x^{(k)})^T \right] \]
where \( s_w^{(k)} = D^{(k)} w^{(2)}/\sqrt{N} \) with \( D^{(k)} = \text{diag} \left( \sigma'(q_w^{(k)}) \right) \), and \( q_w^{(k)} = W^{(1)} x^{(k)}/\sqrt{d} \).

We will first analyze the matrix
\[
\mathbb{E}_{W^{(1)}|w^{(2)}, X} \left[ s_w^{(k)} (s_w^{(k)})^T \right] = \frac{1}{N} \mathbb{E}_{W^{(1)}|w^{(2)}, X} \left[ \text{diag} \left( \sigma'(q_w^{(k)}) \right) w^{(2)} (w^{(2)})^T \text{diag} \left( \sigma'(q_w^{(k)}) \right) \right].
\]
We note that \( q_w^{(k)} \sim \mathcal{N}(0, (r_x^{(k)})^2) \) for all \( i \),
\[
\mathbb{E}_{W^{(1)}|X} \left[ \sigma'(q_{w,i}^{(k)}) \sigma'(q_{w,i}^{(k)}) \right] = \delta_{ij} \mathbb{E}_{W^{(1)}|X} \left[ \sigma'(q_{w,i}^{(k)})^2 \right] + (1 - \delta_{ij}) \mathbb{E}_{W^{(1)}|X} \left[ \sigma'(q_{w,i}^{(k)})^2 \right] = \delta_{ij} \left( \eta_x^{(k)} - \xi^{(k)} \right) + \xi^{(k)}.
\]
Substituting in (55) and using the definition of \( \bar{I} \), we obtain that
\[
\mathbb{E} \left[ \| I - \bar{I} \|_{op}^2 \right] = \mathbb{E} \left[ \left\| \sum_k \left[ \frac{1}{N} w^{(2)} (w^{(2)})^T \Delta \theta^{(k)} \right] \otimes \frac{1}{d} x^{(k)} (x^{(k)})^T \right\|_{op}^2 \right]
\leq N \sum_k \mathbb{E} \left[ \left\| \left( \frac{1}{N} w^{(2)} (w^{(2)})^T \Delta \theta^{(k)} \right) \otimes \frac{1}{d} x^{(k)} (x^{(k)})^T \right\|_{op}^2 \right]
= \frac{1}{N d^2} \sum_k \mathbb{E} \left[ (\Delta \theta^{(k)})^2 \| x^{(k)} \|^2 \right] \mathbb{E} \left[ \| w^{(2)} \|^2 \right]
\leq \frac{1}{d^2 \alpha_2} \sum_k \sqrt{\mathbb{E} \left[ (\Delta \theta^{(k)})^4 \right]} \sqrt{\mathbb{E} \left[ \| x^{(k)} \|^4 \right]},
\]
where we set \( \Delta \theta^{(k)} = \xi^{(k)} - \alpha \xi/\sigma_x^2 \), and used in the first inequality the triangle inequality, in the second equality that \( \| A \otimes B \|_{op} = \| A \|_{op} \| B \|_{op} \), and the Cauchy-Schwarz inequality in the last line. Note that \( \mathbb{E} (\Delta \theta^{(k)})^4 = o(1) \). We therefore obtain that the right hand side of (56) is \( o(1) \cdot (M/d) = o(1) \), which completes the proof of the lemma. \( \square \)
For the next lemma, recall the matrices $\Sigma, \tilde{\Sigma}$, see (38) and (41).

**Lemma 5.3.** Let Assumptions 2.1, 2.2 and 2.3 hold. Then, in the regime $N, d, M \to \infty$ such that $\gamma_0 = \lim_{d \to \infty} d/M \in (0, \infty)$ and $\beta_1 = \lim_{d \to \infty} N/d$, it holds that $\|\Sigma - \tilde{\Sigma}\|_{op} \to 0$ in probability.

**Remark 5.4.** A similar statement for spherical weights and data was proved in [19, Proposition 3], see also [34, Lemma C.7].

**Proof.** We rewrite $\Sigma, \tilde{\Sigma}$ as
\[
\Sigma = \mathbb{E}_x \left[ \sigma(q) \sigma(q)^T \right],
\]
where $q = W^{(1)}x/\sqrt{d}$, and
\[
\tilde{\Sigma} = \frac{\alpha \xi}{d} W^{(1)}(W^{(1)})^T + (\eta_0 - \xi) I_{N_1} + c \frac{1}{d}(1_{N_1}1_{N_1}^T - I_{N_1}),
\]
where $c$ is an appropriate constant. We calculate the elements in the matrix $\Sigma$ of (57),
\[
\Sigma_{ij} = \mathbb{E}_x [\sigma(q_i)\sigma(q_j)],
\]
where $q_i = \sum_k W^{(1)}_{ik} x_k/\sqrt{d}$ and $\mathbb{E}_x q_i = 0$, since $x$ is centered by assumption. We now apply Lemma 5.5 for each Gaussian bi-vector $(q_i, q_j)$, with the functions $f = g = \sigma$, such that $\varepsilon_{ij} = \mathbb{E}_x [q_i q_j] = \sigma_x^2 \sum_k W^{(1)}_{ik} W^{(1)}_{jk} / d$, and $v_i^2 = \sigma_x^2 \sum_k \left( W^{(1)}_{ik} \right)^2 / d$. Therefore,
\[
\Sigma_{ij} = \theta_{1,i} \theta_{1,j} \frac{\sigma_x^2}{d} \sum_k W^{(1)}_{ik} W^{(1)}_{jk}
\]
\[
+ (\eta_{0,i} - \theta_{1,i}^2) \delta_{ij} + \sigma_x^4 \sum_{l=1}^L a_l(v_i)R_{ij} a_l(v_j) + O(\varepsilon_{ij}^{5/2}) 1_{i\neq j}
\]
where for $i, j \in [N_1]$, we set $R_{ij} = \left( \sum_k W^{(1)}_{ik} W^{(1)}_{jk} / d \right)^2$ if $i \neq j$, $R_{ii} = 0$, and the implied constant in the $O(\cdot)$ term in (59) is uniform in $i, j$. We also set $\theta_{1,i} = \mathbb{E} [\sigma'(v_i z)], \eta_{0,i} = \mathbb{E} [\sigma^2(v_i z)] - \mathbb{E} [\sigma(v_i z)]^2$.

First note that, by Chebyshev’s inequality applied on the square of the norm of each row of the matrix $W^{(1)}$, there exists $t_0 = t_0(\sigma_x^2)$ such that for any $0 < t < t_0$ and all $i$, $P(|v_i - v| \geq t) \leq 2e^{-dt^2/8}$. Taking a union bound we have
that $P(\max_i |v_i - v| > t) \leq 2N_1e^{-dt^2/8}$. Taking $t = \sqrt{\log N_1/d^{1/2-\delta}} = o(1)$, we then have by the Borel–Cantelli lemma that for any $\delta > 0$, and all large $N$,

$$\max_i |v_i - v| < (\log N_1)^{1/2}d^{-1/2+\delta} \ a.s. \quad (60)$$

By assumption $\sigma$ and $\sigma'$ are bounded continuous functions, and together with (60) we obtain that the diagonal matrix $(\eta_{0,i} - \theta_{1,i})\delta_{ij}$ converges in operator norm to $(\eta_0 - \xi)I_{N_1}$, in probability. Similarly, using that the matrix $W^{(1)}(W^{(1)})^T/d$ is a Wishart matrix and therefore possesses an operator norm which is bounded in probability uniformly in $N$, we obtain that the operator norm of the difference $(\alpha\xi - \theta_{1,i}\theta_{1,j}\sigma_{x}^2)W^{(1)}(W^{(1)})^T/d$ converges to 0 in probability as $d \to \infty$. It thus remains to handle the matrices composed of the third terms in (59), and of the error terms $\varepsilon_{ij}^{5/2}$.

We now control the third term $\sum_{l=1}^L a_l(v_i)R_{ij}a_l(v_j)$. Using the analysis in [14], we note that the matrix $R$ is precisely the matrix $W$ in the notation of [14, Proof of Theorem 2.1], hence we have that (see pages 12-20 for the proof details)

$$\|R - \frac{1}{d\alpha^2}(1_{N_1}1_{N_1}^T - I_{N_1})\|_{op} \to 0 \quad (61)$$

in probability. Since the $a_l(v_i)$ are continuous and bounded functions by Lemma 5.5, hence following (60) $a_l(v_i)$ is uniformly bounded for all $l$. We now trivially obtain, using the boundedness in norm of $R$ in probability, that with the matrix $A$ such that $A_{l,j} = a_l(v_i)\delta_{ij}$

$$\|\sum_l A_lRA_l - \sum_l a_l(v)R\|_{op} \to 0, \quad \text{in probability.} \quad (62)$$

We finally turn to the matrix composed of the error terms in (59), that is, we bound the operator norm of the symmetric matrix $B$ with entries $B_{ij} = \varepsilon_{ij}^{5/2} = R_{ij}\varepsilon_{ij}^{1/2}$. By a Chebycheff inequality as above, we obtain that for any $\delta > 0$, $\max_{i\neq j} |\epsilon_{ij}| < d^{-1/2+\delta}$ in probability for all large $d$. Therefore, by Gershgorin’s circle theorem, the operator norm of $B$ is bounded above by $d \cdot d^{-5/4+5\delta/2} = o(1)$, in probability, if $\delta$ is chosen small enough.

5.2 Proof of Theorem 3.8

We will use Theorem A.1. Since the estimator is assumed to be unbiased, we have in the notation of Theorem A.1 that $\psi_\theta(x) = f_\theta(x)$, hence $\nabla_\theta \psi_\theta(x) =$
The Fisher information evaluated on the model (2) given a set of \( M \) i.i.d. measurements \( z^{(i)} \) drawn from the probability \( p(Z^{(i)}|\theta) = \prod_i p(z^{(i)}|\theta) \), is then \( I(\theta) = MA(\theta)/\sigma^2 \), with \( A = A(\theta) \) as in (13). Write the spectral resolution of \( A \) as \( A = U\Lambda U^T \), where \( U \in \mathbb{R}^{P \times P} \) is an orthogonal matrix, and \( \Lambda \) is diagonal with entries the eigenvalues of \( A \), arranged in decreasing order. Then \( \Lambda = \begin{bmatrix} \Lambda_k & 0 \\ 0 & 0 \end{bmatrix} \), where \( k = \text{rank}(A) \) and \( \Lambda_k \) is invertible. Denote by \( \Lambda^{-1} \) the pseudo-inverse of \( \Lambda \), that is \( \Lambda^{-1} = \begin{bmatrix} \Lambda_k^{-1} & 0 \\ 0 & 0 \end{bmatrix} \); we define in the same way \( \Lambda^{-1/2} \). Then, with \( J_\theta(\tilde{x}) := \nabla_\theta f_\theta(\tilde{x}) \), the CR bound reads

\[
B^{\text{ub}} = \frac{\sigma^2}{M} \mathbb{E}_{\theta, \tilde{x}} \left[ \max_{a \in \mathbb{R}^P} \frac{a^T \nabla_\theta f_\theta(\tilde{x}) \nabla_\theta f_\theta(\tilde{x})^T a}{a^T A(\theta) a} \right] = \frac{\sigma^2}{M} \mathbb{E}_{\theta, \tilde{x}} \left[ \max_{b \in \mathbb{R}^P} \frac{b^T U^T J_\theta(\tilde{x}) J_\theta(\tilde{x})^T U b}{b^T \Lambda b} \right] \quad (63)
\]

Now, write \( b = \Lambda^{-\frac{1}{2}} \tilde{b} + b_\perp \), where \( b_\perp = [0_k, \tilde{b}] \) such that \( \tilde{b} \in \mathbb{R}^{(P-k) \times 1} \). Note that, \( \Lambda^{\frac{1}{2}} b = \tilde{b} \). Partition \( U = [U_k, U_\perp] \), with \( U_k \in \mathbb{R}^{k \times P} \). The numerator in (63) is then

\[
b^T U^T J_\theta(\tilde{x}) J_\theta(\tilde{x})^T U b = \tilde{b}^T \Lambda^{-\frac{1}{2}} U^T J_\theta(\tilde{x}) J_\theta(\tilde{x})^T U \Lambda^{-\frac{1}{2}} \tilde{b} + 2 \tilde{b}^T U_\perp^T J_\theta(\tilde{x}) J_\theta(\tilde{x})^T U \Lambda^{-\frac{1}{2}} \tilde{b} + \tilde{b}^T U_\perp^T J_\theta(\tilde{x}) J_\theta(\tilde{x})^T U_\perp \tilde{b}
\]

\[
= \tilde{b}^T \Lambda^{-\frac{1}{2}} U^T J_\theta(\tilde{x}) J_\theta(\tilde{x})^T U \Lambda^{-\frac{1}{2}} \tilde{b}, \quad (64)
\]

where the last equality is because the columns of \( J_\theta(\tilde{x}) \) almost surely belong to the span of \( A(\theta) = \mathbb{E}_x J_\theta(\tilde{x}) J_\theta(\tilde{x})^T \), and in particular are orthogonal to the rows of \( U_\perp^T \). Substituting (64) back in (63) we obtain that

\[
B^{\text{ub}} = \frac{\sigma^2}{M} \mathbb{E}_{\theta, \tilde{x}} \left[ \max_{b \in \mathbb{R}^P} \frac{\tilde{b}^T \Lambda^{-\frac{1}{2}} U^T J_\theta(\tilde{x}) J_\theta(\tilde{x})^T U \Lambda^{-\frac{1}{2}} \tilde{b}}{\| \tilde{b} \|^2} \right] = \frac{\sigma^2}{M} \mathbb{E}_\theta \left[ \text{Tr} \left( A \Lambda^{-\frac{1}{2}} \Lambda^{-\frac{1}{2}} U^T \right) \right]
\]

\[
= \frac{\sigma^2}{M} \mathbb{E}_\theta \left[ \text{Tr} \left( U \begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix} U^T \right) \right] = \frac{\sigma^2}{M} \mathbb{E}_\theta \left[ k \right] = \frac{\sigma^2}{M}. \quad (27)
\]
(In the last display, we used that the matrix $\Lambda^{-\frac{1}{2}}U^T J_\theta(\tilde{x})J_\theta(\tilde{x})^T U \Lambda^{-\frac{1}{2}}$ is of rank one in the first equality; in the next to last, we used that $A = U \Lambda U^T$.)

5.3 An auxiliary lemma

**Lemma 5.5.** Let $(q_1, q_2)$ be a bi-variate centered Gaussian vector, with covariance matrix $C = \begin{bmatrix} v_1^2 & \varepsilon \\ \varepsilon & v_2^2 \end{bmatrix}$, such that $\varepsilon < v_i^2$, $i = 1, 2$, and $v_i > 1/2$. Given functions $f_i : \mathbb{R} \rightarrow \mathbb{R}$ with bounded derivatives up to fifth order, we have that

$$
\mathbb{E}[f_1(q_1)f_2(q_2)] = \mathbb{E}[f_1(v_1 z)] \mathbb{E}[f_2(v_2 z)] + \varepsilon \mathbb{E}[f_1'(v_1 z)] \mathbb{E}[f_2'(v_2 z)] + \varepsilon^2 M_{f_1, f_2} + O(\varepsilon^{5/2}),
$$

where $z \sim \mathcal{N}(0, 1)$, $M_{f_1, f_2} = \sum_{\ell=1}^L a_{\ell, f_1}(v_1) b_{\ell, f_2}(v_2)$ with $L < 20$, and the constants $a_{\ell, f_1}(v_1), b_{\ell, f_2}(v_2)$ as well as the implied constant in the $O$ term are bounded by an absolute constant independent of $v_i, \varepsilon$, and the constants $a_{\ell, f_2}$ and $b_{\ell, f_2}$ are continuous in $v_i$.

(The constant $L < 20$ is just a finite constant which we do not bother to make explicit.)

**Proof.** Using the assumption $\varepsilon < v_i^2$, we can represent $q_i$ as

$$q_i = \sqrt{(v_i^2 - \varepsilon)G_i} + \sqrt{\varepsilon}G = v_i G_i + Q_i,$$

with

$$Q_i = \sqrt{\varepsilon}G - c_{\varepsilon,i}G_i, \quad c_{\varepsilon,i} = v_i(1 - \sqrt{v_i^2 - \varepsilon}) = \frac{\varepsilon}{2v_i} + O(\frac{\varepsilon^2}{v_i^3}),$$

where $G_1, G_2, G$ are iid standard centered Gaussians. Using a Taylor expansion to fifth order, we write

$$f_i(q_i) = f_i(v_i G_i) + Q_i f'_i(v_i G_i) + \ldots + \frac{Q_i^4}{4!} f^{(4)}_i(v_i G_i) + \frac{Q_i^5}{5!} f^{(5)}_i(\zeta_i),$$

with $|\zeta_i - v_i G_i| \leq Q_i$. Note that $\mathbb{E}|Q_i|^5 = O(\varepsilon^{5/2})$.

By Gaussian integration by parts, $\mathbb{E}(G_i g(v_i G_i)) = v_i g'(v_i G_i)$ for continuously differentiable functions $g$ that are bounded with their derivative.
Using the fact that \( c_{\varepsilon,i} = \varepsilon/2v_i + O(\varepsilon^2/v_i^2) = \varepsilon/2v_i + O(\varepsilon^3) \), and the Taylor expansion, and writing \( \hat{f}_i = f_i(v_i G_i) \), \( \hat{f}_i' = f_i'(G_i v_i) \), etc., we obtain that
\[
E f_1(q_1) f_2(q_2) = E \hat{f}_1 E \hat{f}_2 + \varepsilon E \hat{f}_1' E \hat{f}_2' + \varepsilon^2 M_{f_1,f_2} + O(\varepsilon^{5/2}), \tag{66}
\]
where \( M_{f_1,f_2} = \sum_{\ell=1}^L a_{\ell,f_1}(v_1) b_{\ell,f_2}(v_2) \), and \( L < 20 \) is an absolute constant independent of \( v_i, \varepsilon \), and due to the Taylor expansion, the constants \( a_{\ell,f_2} \) and \( b_{\ell,f_2} \) are continuous in \( v_i \) by our smoothness assumption on \( f_i \). This completes the proof of the lemma. \( \square \)

### A Background: the Cramér-Rao lower bounds

In this section, we review the Cramér-Rao bounds. We present first a lower bound on the smallest achievable total variance of an estimator. This bound is based on a variation of the basic Cramér-Rao (CR) bound \([10, 42]\). Here, it is presented in the presence of nuisance parameters \([35]\).

**Theorem A.1.** \([28, \text{Theorem 6.6}]\) Let \( \hat{y}_\theta(\tilde{x}, Z) \) be a square integrable estimator. Suppose that

1. \( \psi_\theta(\tilde{x}) = E_{Z|\theta, \tilde{x}} \psi \) and its derivative exist.
2. \( \frac{\partial p(Z|\theta)}{\partial \theta_i} \) exists and square integrable for all \( i \).

Define the likelihood function \( l(Z|\theta) = \log p(Z|\theta) \). Then, \( E_{Z|\theta} \left[ \frac{\partial l(Z|\theta)}{\partial \theta_i} \right] = 0 \), and
\[
E_{\tilde{x}, \theta} \text{Var}_{Z|\theta, \tilde{x}} \hat{y} \geq E_{\tilde{x}} \left[ \max_{\alpha \in \mathbb{R}^P} \frac{\alpha^T \nabla_\theta \psi_\theta(\tilde{x}) (\nabla_\theta \psi_\theta(\tilde{x}))^T \alpha}{\alpha^T I(\theta) \alpha} \right], \tag{67}
\]
where the \( P \times P \) Fisher information matrix \( I(\theta) \) is defined by
\[
I_{ij}(\theta) = E_{Z|\theta} \left[ \frac{\partial l(Z|\theta)}{\partial \theta_i} \frac{\partial l(Z|\theta)}{\partial \theta_j} \right], \quad i, j = 1, \ldots, P. \tag{68}
\]

**Remark A.2.** The formulation of Theorem 6.6 in \([28]\) assumes that the Fisher information \( I \) is invertible. The proof of the theorem is based on Theorem 6.1 there. To obtain the version quoted above, one extends Theorem 6.1 by using the display below (6.4) without the right most equality, and then repeats the proof of Theorem 6.6. Note that when \( I \) is invertible, Theorem A.1 is a reformulation of \([28, \text{Theorem 6.6}]\).
Using the Van Trees (posterior) \[18, 20, 18\] version of the Cramér-Rao inequality for multidimensional parameter space, one can derive a lower bound on the generalization error of a possibly biased estimators \( \hat{y}_\theta(\tilde{x}, Z) \). We provide here a version of this inequality, where we condition over part of the parameters’ space:

**Theorem A.3.** (\[20, Theorem 1\]) Let \( \hat{y}_\theta(\tilde{x}, Z) \) be an estimator of \( f_\theta(\tilde{x}) \). Partition \( \theta = (\theta_c, \theta_l) \in \mathbb{R}^P \), where \( \theta_c \in \mathbb{R}^{N_c} \), and \( \theta_l \in \mathbb{R}^{N_l} \), such that \( P = N_c + N_l \). Suppose that,

1. The functions \( f_\theta(\tilde{x}) \), \( \nabla_{\theta_c} f_\theta(\tilde{x}) \) are absolutely continuous in \( \theta_c \) for almost all values of \( \theta_c \).

2. \( p(y, \theta_c|\theta_l, X) \) is Gaussian. (As in \[2\].)

3. \( \theta_c \sim \mathcal{N}(0, \alpha^{-1} I_{N_c}) \) is independent of \( \theta_l \)

4. The Fisher information, \( I_\alpha(\theta_l, X) \in \mathbb{R}^{N_c \times N_c} \) exists and \( \text{diag}(I_\alpha(\theta_l, X))^{1/2} \) is locally integrable in \( \theta_c \), where

\[
I_\alpha(\theta_l, X) = \sum_{k=1}^{M} \mathbb{E}_{\theta_c|\theta_l, X} \left[ \nabla_{\theta_c} f_\theta(\tilde{x}^{(k)}) \left( \nabla_{\theta_c} f_\theta(\tilde{x}^{(k)}) \right)^T \right] + \alpha I_{N_c}. \tag{69}
\]

Then, with \( J(\theta_l, \tilde{x}) = \mathbb{E}_{\theta_c|\theta_l, \tilde{x}} \nabla_{\theta_c} f_\theta(\tilde{x}) \), we have that

\[
\mathbb{E}(\hat{y} - f_\theta(\tilde{x}))^2 \geq \mathbb{E}_{\theta_l, \tilde{x}, X} \left[ J(\theta_l, \tilde{x})^T (I_\alpha(\theta_l, X))^{-1} J(\theta_l, \tilde{x}) \right]. \tag{70}
\]

**Remark A.4.** \[20\] Theorem 1] is presented in more general settings and for more general distribution \( p(Y, \theta_c|\theta_l, X) \). Theorem A.3 is derived from \[20\], Theorem 1] by taking \( C = J(\theta_l, \tilde{x})^T (I_\alpha(\theta_l, X))^{-1} \in \mathbb{R}^{1 \times N_c} \) independent on \( \theta_c \) and \( B = 1 \). Also, in our setting, we condition on the features, \( X \), and part of the parameters space, \( \theta_l \), and take the expectation only over the measurement noise and \( \theta_c \). We further note that \[20\], Theorem 1] requires \( \theta \) to be in compact support. This assumption can be relaxed to include the Gaussian case, see for example \[18\] Theorem 1].

**Remark A.5.** Different partitions of the parameters’ space may provide different bounds, the choice of the best bound depends on the specific structure of the problem \[9\].
Using Theorem A.3, we provide the following bound which utilizes the layered structure of feed-forward networks.

**Corollary A.6.** Setup as in Theorem A.3. Let \( f_{\theta}(\tilde{x}) \) be as in (3) and let Assumption 2.2 hold. Then,

\[
E_g \geq \max_{l \in [1, L]} B^{(l)},
\]

(71)

with

\[
B^{(l)} := \mathbb{E}_{\theta_l, \tilde{x}, X} \left[ J(\theta_l, \tilde{x})^T (I^{(l)}_\alpha(\theta_l, X))^{-1} J(\theta_l, \tilde{x}) \right],
\]

(72)

where \( J(\theta_l, \tilde{x}) = (\mathbb{E}_{W^{(l)}|\theta_l, \tilde{x}} \nabla_{W^{(l)}} f_{\theta}(\tilde{x})) \), \( \theta_l \) are the parameters of the network without the \( l \)th layer \( W^{(l)} \), and the conditional Fisher matrix \( I^{(l)}_\alpha(\theta_l, X) \in \mathbb{R}^{N_l N_{l-1} \times N_l N_{l-1}} \) is

\[
I^{(l)}_\alpha(\theta_l, X) = \sum_{k=1}^M \mathbb{E}_{W^{(l)}|\theta_l, X} \left[ \nabla_{W^{(l)}} f_{\theta}(x_k) \left( \nabla_{W^{(l)}} f_{\theta}(x_k) \right)^T \right] + \alpha_l I_{N_l N_{l-1}},
\]

(73)

**Proof.** Apply Theorem A.3 \( L \) times: for a given \( l \), choose \( \theta_c = W^{(l)} \), and \( \theta_l \) to be the remaining parameters of the model, and then take the best over all bounds. Substitution in (69) yields (73). \( \Box \)

### B Unbiased estimator - examples

In this section, we specialize Theorem 3.8 to various network architectures. Auxiliary results concerning the structure of the Fisher information matrix are collected in Section C. As we will see, nonlinear models exhibit a much higher rank of the Fisher information matrix.

#### B.1 Linear activation function

**Corollary B.1.** Consider the model in (2), (3) with \( \sigma(x) = x \), \( N_L = 1 \) and \( L \geq 1 \) layers. Assume that \( p(\theta) \) has finite covariance matrix. Let \( \hat{y}(\tilde{x}, Z) \) be any unbiased square integrable estimator. Then

\[
\mathbb{E} (\tilde{y} - \hat{y})^2 \geq \frac{\sigma^2}{M} \text{Rank} (\Sigma), \quad \Sigma = \mathbb{E} [xx^T].
\]

(74)
Proof. We again apply theorem 3.8. By (14), we need to calculate the rank of the Fisher matrix \( I(\theta) \), see (13), for \( f_\theta(x) \) defined in (3) with \( \sigma(x) = x \). By Lemma C.1 below, the Fisher matrix can be written as

\[
I(\theta) = M_\sigma^2 \left( \prod_{l=1}^{L} \frac{1}{N_l} \right) J_L J_L^T,
\]

where the matrix, \( J_L \in \mathbb{R}^{P \times d N_L} \) is defined in (82). Taking \( N_L = 1 \), we have that, 

\[
E_{\theta} \left[ \text{Rank}(I(\theta)) \right] = \text{Rank}(I(\theta)) = \text{Rank}(J_L) = d,
\]

since \( P > d \), which completes the proof. \( \square \)

B.2 Nonlinear activation function

Matrix rank is unstable with respect to perturbations. As we now show, even weak non-linearities generate small eigenvalues in the Fisher matrix, and increases dramatically its rank.

**Theorem B.2.** Consider the model in (2), (3) with \( L = 2 \), and let Assumptions 2.1, 2.2 and 2.3 hold, with activation function \( \sigma \) satisfying \( \eta_1 > \xi \), i.e., the function \( \sigma' \) is not identically constant. In the regime \( N_1, d \rightarrow \infty \) such that \( \beta_1 = \lim_{d \rightarrow \infty} N_1/d \in (0, \infty) \), we have that 

\[
E_{\theta} \left[ \text{Rank}(I(\theta)) \right] = \beta_1 d^2 (1 + o(1)),
\]

where \( I(\theta) \) is as in (13).

**Remark B.3.** The same proof, using the recursive structure of the function \( f_\theta \), shows that the conclusion of Theorem B.2 hold for any \( L \geq 2 \).

**Remark B.4.** It follows in particular that in the asymptotic regime described in Theorem B.2, the generalization error of any unbiased estimator is worse than the Bayesian error. While somewhat counter-intuitive, it is consistent with the fact that in general, biased estimators can sometimes achieve a lower error than the CR bound for unbiased estimator. For example, a better bound can be achieved for biased estimators by taking the lowest bias, see [7].

**Proof.** We work in the regime where \( \beta_1 = \lim_{d \rightarrow \infty} N_1/d \in (0, \infty) \). Recall the definition of \( f_\theta(x) = (w^{(2)})^T \sigma(q)/\sqrt{N} \), where \( q = W^{(1)} x/\sqrt{d} \), see (3) with \( L = 2, N_1 = N \) and \( N_2 = 1 \) of gradient

\[
J_\theta(\tilde{x}) := \nabla_\theta f_\theta(\tilde{x}) = \begin{bmatrix} \nabla_{W^{(1)}} f_\theta(x) \\ \nabla_{w^{(2)}} f_\theta(x) \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{d}} s_{w}^1 \otimes x \\ \frac{1}{\sqrt{N}} \sigma(q) \end{bmatrix}
\]

where \( s_{w}^1 = D^1 w^{(2)}/\sqrt{N} \in \mathbb{R}^N \), with \( D^1 = \text{diag}(\sigma'(q)) \). The Fisher information matrix for the model in (2) as defined in (13) has the following
form:

\[
A = \mathbb{E}_x \left[ J_\theta(x) J_\theta(x)^T \right] \\
= \frac{1}{N} \left[ \beta_1 \mathbb{E}_x \left[ (s_w^1 \otimes x)(x^T \otimes s_w^1)^T \right] + \beta_2 \mathbb{E}_x \left[ (s_w^1 \otimes x)\sigma(q)^T \right] \right] \\
=: \begin{bmatrix} A^{(1)} \in \mathbb{R}^{Nd \times Nd} & A^{(2)} \in \mathbb{R}^{Nd \times N} \end{bmatrix} \\
A^{(3)} \in \mathbb{R}^{N \times N}
\]

For the lemma, we only care about \( A^{(1)} = \frac{1}{dN} A_R \) the top \( Nd \times N \) block of \( A(\theta) \), where

\[
A_R = \mathbb{E}_x \left[ D^1 w^{(2)}(w^{(2)})^T D^1 \otimes xx^T \right].
\]

Using Lemma C.3, the matrix \( A_R(\theta) \) can be rewritten as

\[
A_R = D^{(2)} \otimes I_d + B + \mathcal{E}_w
\]

such that \( \text{Rank}(B) = o(Nd) \), and \( \|\mathcal{E}_w\|_{\text{HS}} = o(Nd) \) in probability. The matrix \( D^{(2)} \in \mathbb{R}^{N \times N} \) is a diagonal matrix, where the \( (i,j) \) element is \( D^{(2)}_{ij} = \delta_{ij} \sigma^2 w_i w_j ^2 \). The constants \( a_i = \eta_{1,i} - \theta_{1,i} > 0 \) by assumption for all \( i \in [1, N_1] \) and are independent of the vector \( w^{(2)} \). Using spectral decomposition, the matrix \( \mathcal{E}_w \) can be decomposed as \( \mathcal{E}_w = \mathcal{E}_{w1} + \mathcal{E}_{w2} \), such that \( \text{Rank}(\mathcal{E}_{w1}) = o(N_1d) \), and \( \|\mathcal{E}_{w2}\|_{\text{op}} \to 0 \). Hence, we can write

\[
A_R = D^{(2)} \otimes I_d + B + \mathcal{E}_w
\]

such that \( \mathcal{B} = B + \mathcal{E}_{w1} \), where \( \text{Rank}(\mathcal{B}) = o(Nd) \). We will now bound the eigenvalues of \( A_R(\theta) \) from below to estimate its rank. Define the events \( \mathcal{A}_\varepsilon = \{\|\mathcal{E}_{w2}\|_{\text{op}} \leq \varepsilon\} \) and \( \mathcal{B}_\delta = \{\# \{i \in 1, \ldots, N : (a_i w_i ^2)^2 < 2\varepsilon\} > \delta N\} \).

We know that \( \mathbb{P}(\mathcal{A}_\varepsilon) \to 1 \). We now note, using the Gaussian density of the \( w_i ^2 \)s, that

\[
\mathbb{P}(\mathcal{B}_\delta) \leq \frac{N\mathbb{P}(a_i w_i ^2 < 2\varepsilon)}{\delta N} \leq c_1 \frac{\sqrt{\varepsilon}}{\delta}
\]

with some fixed constant \( c_1 > 0 \). Taking \( \delta = \varepsilon^{1/4} \), we thus conclude that \( \mathbb{P}(\mathcal{B}_{\varepsilon^{1/4}}) \to 0 \), and therefore \( \mathbb{P}(\mathcal{B}_{\varepsilon^{1/4}} \cap \mathcal{A}_\varepsilon) \to 1 \). On the event \( \mathcal{B}_{\varepsilon^{1/4}} \cap \mathcal{A}_\varepsilon \), we have that \( \# \{i : a_i w_i ^2 \geq 2\varepsilon\} \geq (1 - \varepsilon^{1/4})Nd \), and also \( \|\mathcal{E}_{w2}\|_{\text{op}} \leq \varepsilon \). Thus, using Weyl’s inequality and the fact that \( \text{Rank}(\mathcal{B}) = o(N_1d) \), on this event \( \text{Rank}(A_R(\theta)) \geq (1 - 2\varepsilon^{1/4})Nd \), for large \( N \). The expected rank is then bounded from below, for large \( N \), by

\[
\mathbb{E}_\theta [\text{Rank}(A_R)] \geq (1 - 2\varepsilon^{1/4})Nd \mathbb{P}(\mathcal{B}_{\varepsilon^{1/4}} \cap \mathcal{A}_\varepsilon) \geq (1 - 2\varepsilon^{1/4})Nd(1 - o(1)).
\]
We thus conclude that $\mathbb{E}_\theta [\text{Rank}(A_R(\theta))] = (1 - o(1))\beta_1 d^2$. Now, note that the rank of $A_R(\theta)$ bounds from below the rank of $A(\theta)$, and therefore, $\mathbb{E}_\theta [\text{Rank}(I(\theta))] \geq \beta_1 d^2(1 - o(1))$, which completes the proof. 

\section{Structure of the Fisher information matrix of a feed-forward neural network}

In this section, we analyze the structure of the Fisher information matrix of feed-forward networks; Lemma \ref{lem:linear_structure} considers linear activation functions and any number of layers, while Lemma \ref{lem:nonlinear_structure} considers two layered networks with nonlinear activation functions. This analysis is then used in calculating the expected rank of the Fisher information in Corollary \ref{cor:expected_rank} and Theorem \ref{thm:expected_rank}.

\begin{lemma}
Suppose $\mathbb{E} xx^T = \Sigma$, then the matrix defined in (13) with $f_\theta(x)$ as in (3) and $\sigma(x) = x$ can be decomposed as

$$I_1 = \left( \prod_{l=1}^{L} \frac{1}{N_{l-1}} \right) J_L J_L^T$$

such that, the matrix $J_L \in \mathbb{R}^{P \times dN_L}$ is composed of $L$ blocks where the $l$th block is $J_l^L = B_l^T \otimes A_l \Sigma^{1/2} \in \mathbb{R}^{N_l N_{l-1} \times dN_L}$, and

$$B_l^T = \begin{cases} I_{N_L} & l = L \\ W^{(L)} & l = L - 1 \\ \Pi_{m=L}^{l+1} (W^{(m)})^T & 1 \leq l < L - 1 \end{cases},$$

and

$$A_l = \begin{cases} I_d & l = 1 \\ \Pi_{m=1}^{l-1} W^{(m)} & 1 \leq l \leq L \end{cases}.$$ \label{eq:structure1}

\end{lemma}

\begin{remark}
Similar results are derived for $L = 2$ in \cite{41}). Here, we consider general $L$.
\end{remark}

\begin{proof}
We use (13) with the following model for a deep neural network with linear activation (3):

$$f_\theta(x) = \left( \prod_{l=1}^{L} \frac{1}{\sqrt{N_{l-1}}} W^{(l)} \right) x$$

\end{proof}
The Fisher matrix is of size $P \times P$, where $P = \sum_{i=1}^{L} N_i N_{i-1}$ is the total number of parameters. It is composed of blocks,

$$
I_1 = \mathbb{E}_x \begin{bmatrix}
J^{(1)}(J^{(1)})^T & J^{(1)}(J^{(2)})^T & \cdots & J^{(1)}(J^{(L)})^T \\
J^{(2)}(J^{(1)})^T & J^{(2)}(J^{(2)})^T & \cdots & J^{(2)}(J^{(L)})^T \\
\vdots & \vdots & \ddots & \vdots \\
J^{(L)}(J^{(1)})^T & J^{(L)}(J^{(2)})^T & \cdots & J^{(L)}(J^{(L)})^T 
\end{bmatrix},
$$

(85)

where $J^{(l)}$, the Jacobean matrix of $l$th layer is defined as follow, for $1 \leq l < L$:

$$
J^{(l)} = \nabla_{W^{(1)}} f_\theta(x) = \prod_{m=L}^{l+1} (W^{(m)})^T \otimes \prod_{m=1}^{L} W^{(m)} x \in \mathbb{R}^{N_{l-1} \times N_i}.
$$

(86)

We rewrite this matrix as follows:

$$
J^{(l)} = B_l^T \otimes A_l x \in \mathbb{R}^{N_{l-1} \times N_i \times d_{N_L}}
$$

where $A_l \in \mathbb{R}^{N_{l-1} \times d}$, and $B_l \in \mathbb{R}^{N_i \times N_l}$, are defined in (84) and (83). The $(l,m)$th block of the Fisher matrix in (85):

$$
\mathbb{E}_x J^{(l)}(J^{(m)})^T = B_l^T B_m \otimes A_l \mathbb{E}_x x^T A_m^T = \sigma_x^2 B_l^T B_m \otimes A_l \Sigma A_m^T
$$

$$
= (B_l^T \otimes A_l \Sigma^{1/2}) (B_m \otimes \Sigma^{1/2} A_m^T) = \sigma_x^2 J_L^{(l)}(J_L^{(m)})^T
$$

(87)

Denoting by $J_L^{(l)} = B_l^T \otimes A_l \Sigma^{1/2} \in \mathbb{R}^{N_{l-1} \times d_{N_L}}$. Substituting (87) for all blocks in (85) yield the desired result, i.e., the Fisher matrix for linear activation function can be written as follows:

$$
I_1 = \left( \prod_{l=1}^{L} \frac{1}{N_{l-1}} \right) J_L J_L^T,
$$

(88)

such that the matrix $J_L \in \mathbb{R}^{P \times d_{N_L}}$ is composed of $L$ blocks where the $l$th block is $J_L^{(l)}$.

Lemma C.3. Let Assumptions 2.1, 2.2 and 2.3 hold. Let $A_R$ be as in (77). Then, with $\beta_1 = \lim_{d \to \infty} N/d \in (0, \infty)$, there exist matrices $D^{(2)}$, $B$ and $E_w$ such that

$$
A_R = D^{(2)} \otimes I_d + B + E_w,
$$

(89)

with

1. $\text{Rank}(B) = o(d^2)$

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Proof of Lemma C.3. Each element in the matrix $A_R$ is of the following form:

$$A_{R,(i_1,i_2;i'_1,i'_2)} = w^{(2)}_{i_2} w^{(2)}_{i_2} \mathbb{E}_x [\sigma'(q_{i_2}) \sigma'(q_{i'_2}) x_{i_1} x_{i'_1}] .$$

Set $\bar{q}_{i_2} = \frac{1}{\sqrt{d}} \sum_{i \neq i_1,i'_1} W^{(1)}_{ij} x_i$, and $\bar{q}_{i_2} = \frac{1}{\sqrt{d}} \sum_{i \neq i_1,i'_1} W^{(1)}_{i_{2}} x_i$. Using a Taylor expansion of the function $\sigma'$ around these points up to third order, we have that for any $i_2, i'_2$ and $i_1 = i'_1$,

$$\mathbb{E}_x [\sigma'(q_{i_2}) \sigma'(q_{i'_2}) x_{i_1}^2] = \sigma^2_x M^{(1)}_{i_2 i'_2}$$

$$+ \frac{6 \sigma_x^4}{d} (M^{(2)}_{i_2 i'_2} W^{(1)}_{i_{2} i_{2} i_{1}} + M^{(13)}_{i_2 i'_2} W^{(1)}_{i_{2} i_{2} i_{1}})^2 + M^{(13)}_{i_2 i'_2} W^{(1)}_{i_{2} i_{2} i_{1}} + \mathcal{E}_{(i_2,i'_2,i_1,i'_1)}$$

(90)

and for any $i_2, i'_2$ and $i_1 \neq i'_1$,

$$\mathbb{E}_x [\sigma'(q_{i_2}) \sigma'(q_{i'_2}) x_{i_1} x_{i'_1}] = \sigma^4_x d^{-1} (M^{(2)}_{i_2 i'_2} W^{(1)}_{i_{2} i_{2} i_{1}} + W^{(1)}_{i_{2} i_{2} i_{1}})$$

$$+ \frac{6 \sigma_x^4}{d} (M^{(13)}_{i_2 i'_2} W^{(1)}_{i_{2} i_{2} i_{1}} + M^{(13)}_{i_2 i'_2} W^{(1)}_{i_{2} i_{2} i_{1}} + \mathcal{E}_{(i_1,i_2,i'_1,i'_2)}$$

(91)

where we define $M^{(1)}_{i_2 i'_2} = \mathbb{E}_x [\sigma'(\bar{q}_{i_2}) \sigma'(\bar{q}_{i'_2})]$, $M^{(2)}_{i_2 i'_2} = \mathbb{E}_x [\sigma''(\bar{q}_{i_2}) \sigma''(\bar{q}_{i'_2})]$, and $M^{(13)}_{i_2 i'_2} = \mathbb{E}_x [\sigma'(\bar{q}_{i_2}) \sigma''(\bar{q}_{i'_2})]$. The matrix $\mathcal{E}$ is the remaining terms of order $d^{-3/2}$, i.e. $\mathbb{E}_x \mathcal{E}_{(i_2,i'_2,i_1,i'_1)} \leq C/d^3$. To evaluate the $M''$ matrix elements we apply Lemma 5.5 with $\bar{q}_{i_2 i'_2} = \sigma^2_x/d \sum_{k \neq i_1,i'_1} W^{(1)}_{i_{2}k} W^{(1)}_{i_{2} k}$ and $\tilde{v}_{i_2}^2 = \sigma^2_x/d \sum_{k \neq i_1,i'_1} (W^{(1)}_{i_{2}k})^2$ for $i = i_2, i'_2$. We will now expand the typical matrix elements in the four following cases; in each case, the matrix $\tilde{\mathcal{E}}$ satisfies conditions as noted:

1. $i_2 \neq i'_2$ and $i_1 = i'_1$

$$\mathbb{E}_x [\sigma'(q_{i_2}) \sigma'(q_{i'_2}) x_{i_1}^2] = \sigma^2_x (\theta_{1,i'_2} \theta_{1,i_2} + \theta_{2,i,i'_2} \theta_{2,i'_2}) \sigma^2_x \sum_{k \neq 1} W^{(1)}_{i_{2}k} W^{(1)}_{i_{2} k} + O(\sigma^2_x x_{i_2 i'_2}))$$

$$+ \frac{6 \sigma_x^4}{d} \left( \theta_{1,i'_2} \theta_{1,i_2} W^{(1)}_{i_{2} i_{2} i_{1}} + \theta_{1,i'_2} \theta_{1,i_2} (W^{(1)}_{i_{2} i_{2} i_{1}})^2 + \theta_{2,i,i'_2} \theta_{2,i'_2} (W^{(1)}_{i_{2} i_{2} i_{1}})^2 + \mathcal{E}_{(i_1,i_2,i'_1,i'_2)} \right)$$

$$= \sigma^2_x \theta_{1,i'_2} \theta_{1,i_2} + \tilde{\mathcal{E}}_{(i_1,i_2,i'_1,i'_2)} ,$$

(92)

with $\mathbb{E}({\tilde{\mathcal{E}}}_{(i_1,i_2,i'_1,i'_2)}) \leq C/d^2$. 

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2. \( i_2 \neq i_2' \) and \( i_1 \neq i_1' \)

\[
\mathbb{E}_x \left[ \sigma'(q_{i_2}) \sigma'(q_{i_2'}) x_i x_i' \right] = \frac{\sigma_x^4}{d} \theta_{2,i_2} \theta_{2,i_2'} (W_{i_2'i_1}^{(1)} W_{i_2'i_1'}^{(1)} + W_{i_2'i_1}^{(1)} W_{i_2'i_1'}^{(1)})
\]

\[
+ \frac{\sigma_x^4}{d} (\theta_{3,i_2} \theta_{1,i_2} W_{i_2'i_1}^{(1)} W_{i_2'i_1}^{(1)} + \theta_{3,i_2} \theta_{1,i_2'} W_{i_2'i_1}^{(1)} W_{i_2'i_1'}^{(1)}) + \tilde{\mathcal{E}}_{(i_1,i_2,i_1',i_2')}.
\]

(93)

where the matrix element \( \tilde{\mathcal{E}}_{(i_1,i_2,i_1',i_2')} \) is the matrix element \( \mathcal{E}_{(i_1,i_2,i_1',i_2')} \) plus higher order terms, whose second moment is bounded by \( C/d^3 \), and therefore \( \mathbb{E}(\tilde{\mathcal{E}}_{(i_1,i_2,i_1',i_2')}) \leq C/d^3 \).

3. \( i_2 = i_2' \) and \( i_1 = i_1' \)

\[
\mathbb{E}_x \left[ \sigma'(q_{i_2})^2 x_i^2 \right] = \sigma_x^2 \eta_{1,i_2} + \frac{6\sigma_x^4}{d} (W_{i_2'i_1}^{(1)})^2 (\eta_{2,i_2} + 2\eta_{31,i_2}) + \mathcal{E}_{(i_1,i_2,i_1',i_2')} = \sigma_x^2 \eta_{1,i_2} + \tilde{\mathcal{E}}_{(i_1,i_2,i_1',i_2')}.
\]

(94)

with \( \mathbb{E}(\tilde{\mathcal{E}}_{(i_1,i_2,i_1',i_2')}) \leq C/d^2 \).

4. \( i_2 = i_2' \) and \( i_1 \neq i_1' \)

\[
\mathbb{E}_x \left[ \sigma'(q_{i_2})^2 x_i x_i' \right] = \frac{2\sigma_x^4}{d} \eta_{2,i_2} W_{i_2'i_1}^{(1)} W_{i_2'i_1'}^{(1)}
\]

\[
+ \frac{2\sigma_x^4}{d} \eta_{31,i_2} W_{i_2'i_1}^{(1)} W_{i_2'i_1'}^{(1)} + \mathcal{E}_{(i_2,i_2',i_1,i_1')} = \tilde{\mathcal{E}}_{(i_2,i_2',i_1,i_1')}.
\]

(95)

with \( \mathbb{E}(\tilde{\mathcal{E}}_{(i_1,i_2,i_1',i_2')}) \leq C/d^2 \).

Combining (92), (93), (94), and (95), and rearranging the elements in a matrix form we can now rewrite the matrix \( A_R \) as

\[
A_R = D^{(2)} \otimes I_d + B + \mathcal{E}_w,
\]

(96)

where \( D^{(2)} \) is a block diagonal matrix of size \( N_1 \) whose \((i,j)\)th element is

\[
D_{ij}^{(2)} = \delta_{ij} \sigma_x^2 (\eta_{1,j} - \theta_{1,j}^2) (w_i^{(2)})^2,
\]

and

\[
B = J_w^T \theta_1 \otimes A + \theta_1^T \otimes A^T + R_w R_w^T + C_w C_w^T.
\]

(97)

The vector \( J_w = (\theta_2 \circ w^{(2)}) \otimes I_d \), and \( \theta_{k,i} \) is the \( i \)th element in the vector \( \theta_k \in \mathbb{R}^{N_1} \) for \( k = 1, 2 \). The matrix \( A \in \mathbb{R}^{d \times d N_1} \) is a block matrix, composed of \( N_1 \) blocks of size \( d \times d \). The \((i,j)\)th element in the block \( k \) is
The vector $R_w, C_w \in \mathbb{R}^{N_1d}$ is composed of the rows and the columns of the matrix $\sigma_x^4 W(1)/d$, arranged in a vector Hadamard product with the vector $\theta_2$, respectively. Therefore, $\text{Rank}(B) \leq N + d + 2$, since $\text{Rank}(\theta_1 \otimes A) = \text{Rank}(A) = d$. The matrix $E_w$ has elements $E_{w,i_2,i_1,i_1'} = E_{i_2,i_1,i_1'}^w$. Note that our estimates on the individual entries of $E_w$ imply that $\mathbb{E} \left[ \| \tilde{E}_w \|_{\text{HS}}^2 \right] \leq Cd$ for some positive constant $C > 0$. This completes the proof of the lemma.

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