On the Variance of the Fisher Information for Deep Learning*

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Abstract

In the realm of deep learning, the Fisher information matrix (FIM) gives novel insights and useful tools to characterize the loss landscape, perform second-order optimization, and build geometric learning theories. The exact FIM is either unavailable in closed form or too expensive to compute. In practice, it is almost always estimated based on empirical samples. We investigate two such estimators based on two equivalent representations of the FIM — both unbiased and consistent. Their estimation quality is naturally gauged by their variance given in closed form. We analyze how the parametric structure of a deep neural network can affect the variance. The meaning of this variance measure and its upper bounds are then discussed in the context of deep learning.

1 Introduction

The Fisher information is one of the most fundamental concepts in statistical machine learning. Intuitively, it measures the amount of information carried by a single random observation when the underlying model varies along certain directions in the parameter space: if such a variation does not change the underlying model, then a corresponding observation contains zero (Fisher) information and is non-informative regarding the varied parameter. Parameter estimation is impossible in this case. Otherwise, if the variation significantly changes the model and has large information, then an observation is informative and the parameter estimation can be more efficient as compared to parameters with small Fisher information. In machine learning, this basic concept is useful for defining intrinsic structures of the parameter space, measuring model complexity, and performing gradient-based optimization.

Given a statistical model that is specified by a parametric form \( p(z \mid \boldsymbol{\theta}) \) and a continuous domain \( \boldsymbol{\theta} \in \mathcal{M} \), the Fisher information matrix (FIM) is a 2D tensor varying with \( \boldsymbol{\theta} \in \mathcal{M} \), given by

\[
\mathcal{I}(\boldsymbol{\theta}) = \mathbb{E}_{p(z \mid \boldsymbol{\theta})} \left( \frac{\partial \ell}{\partial \boldsymbol{\theta}} \frac{\partial \ell}{\partial \boldsymbol{\theta}^\top} \right),
\]

where \( \mathbb{E}_{p(z \mid \boldsymbol{\theta})} (\cdot) \), or simply \( \mathbb{E}_p (\cdot) \) if the model \( p \) is clear from the context, denotes the expectation w.r.t. \( p(z \mid \boldsymbol{\theta}) \), and \( \ell \coloneqq \log p(z \mid \boldsymbol{\theta}) \) is the log-likelihood function. All vectors are column vectors throughout this paper. Under weak conditions (see Lemma 5.3 in Lehmann and Casella [1998] for the univariate case),

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the FIM has the equivalent expression $\mathcal{I}(\theta) = \mathbb{E}_{p(z|\theta)} \left( -\partial^2 \ell / \partial \theta \partial \theta^\top \right)$. Given $N$ i.i.d. observations $z_1, \ldots, z_N$, these two equivalent expressions of the FIM lead to two different estimators

$$\hat{\mathcal{I}}_1(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{\partial \ell_i}{\partial \theta} \frac{\partial \ell_i}{\partial \theta^\top} \right) \quad \text{and} \quad \hat{\mathcal{I}}_2(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left( -\frac{\partial^2 \ell_i}{\partial \theta \partial \theta^\top} \right),$$

(2)

where $\ell_i := \log p(z_i|\theta)$ is the log-likelihood of the $i$'th observation $z_i$. The notations $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ are abused for simplicity as they depend on both $\theta$ and the random observations $z_i$.

These estimators are universal and independent to the parametric form $p(z|\theta)$. They are expressed in terms of the 1st- or 2nd-order derivatives of the log-likelihood. Usually, we already have these derivatives to perform gradient-based learning. Therefore, we can save computational cost and reuse these derivatives to estimate the Fisher information, which in turn can be useful, e.g., to perform natural gradient optimization [Amari, 2016, Pascanu and Bengio, 2014]. Estimating the FIM is especially meaningful for deep learning, where the computational overhead of the exact FIM can be significant.

It is straightforward from the law of large numbers and the central limit theorem that both estimators in Eq. (2) are unbiased and consistent. This is formally stated as follows.

**Proposition 1.**

$$\mathbb{E}_{p(z|\theta)} \left( \hat{\mathcal{I}}_1(\theta) \right) = \mathbb{E}_{p(z|\theta)} \left( \hat{\mathcal{I}}_2(\theta) \right) = \mathcal{I}(\theta),$$

$$\forall \epsilon > 0, \lim_{N \to \infty} \operatorname{Prob} \left( \left\| \hat{\mathcal{I}}_1(\theta) - \mathcal{I}(\theta) \right\|_F + \left\| \hat{\mathcal{I}}_2(\theta) - \mathcal{I}(\theta) \right\|_F > \epsilon \right) = 0,$$

where $\operatorname{Prob}(\cdot)$ denotes the probability of the parameter statement being true and $\| \cdot \|_F$ is the Frobenius norm of a tensor (with $\| \cdot \|_2$ as the regular vector $L_2$-norm).

The Fisher information can be zero for non-regular models or infinite [Chen and Li, 2009]. However, these properties may not be preserved by the empirical estimators.

How far can $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ deviate from the “true FIM” $\mathcal{I}(\theta)$, and how fast can they converge to $\mathcal{I}(\theta)$ as the number of observations increases? To answer these questions, it is natural to think of the variance of $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$. For example, an estimator with a large variance means the estimation does not accurately reflect $\mathcal{I}(\theta)$; and any procedure depending on the FIM consequently suffers from the estimation error. Through studying the variance, we can control the estimation quality and reliably perform subsequent measurements or algorithms based on the FIM.

Towards this direction, we made the following contributions that will unfold in the following Sections 2 to 4:

- We review and rediscover two equivalent expression of the FIM in the context of deep feed-forward networks (Section 2);
- We give in closed form the variance (extending to meaningful upper bounds) and discuss the convergence rate of the estimators $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ (Section 3);
- We analyze how the 1st- and 2nd-order derivatives of the neural network can affect the estimation of the FIM (Section 4).

We discuss related work in Section 5 and conclude in Section 6.

## 2 Feed-forward Networks with Exponential Family Output

This section realizes the concept of Fisher information in a feed-forward network with exponentially family output and explains why its estimators are useful in theory and practice.
Consider supervised learning with a neural network. The underlying statistical model is $p(z \mid \theta) = p(x)p(y \mid x, \theta)$, where $z = (x, y)$, the random variable $x$ represents features, and $y$ is the target variable. The marginal distribution $p(x)$ is parameter-free, usually fixed as the empirical distribution $p(x) = \frac{1}{M} \sum_{i=1}^{M} \delta(x - x_i)$ w.r.t. a set of observations $\{x_i\}_{i=1}^{M}$, where $\delta(\cdot)$ is the Dirac delta. In this paper, we consider w.l.o.g. $M = 1$ as the FIM w.r.t. observations $\{x_i\}_{i=1}^{M}$ is simply the average over FIMs of each individual observation. All results generalize to multiple observations by taking the empirical average.

The predictor $p(y \mid x, \theta)$ is a neural network with parameters $\theta = \{W_{l-1}\}_{l=1}^{L}$ and exponential family output units, given by

$$p(y \mid x) = \exp \left( t^\top(y) h_L - F(h_L) \right),$$
$$h_L = W_{L-1} h_{L-1},$$
$$h_l = \sigma(W_{l-1} h_{l-1}), \quad (l = 1, \ldots, L - 1)$$
$$h_L = (h_L^\top, 1)^\top,$$
$$h_0 = x,$$ (3)

where $t(y)$ is the sufficient statistics of the prediction model, $F(h) = \log \int \exp(t(y)h)dy$ is the log-partition function, and $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ is an element-wise non-linear activation function. Moreover, $W_l$ is a $n_{l+1} \times (n_l + 1)$ matrix, representing the neural network parameters (weights and biases) in the $l$th layer, where $n_l := \dim(h_l)$ denotes the size of layer $l$. We use $W_l^-$ for the $n_{l+1} \times n_l$ weight matrix without the bias terms, obtained by removing the last column of $W_l$. $h_l$ is a learned representation of the input $x$. All intermediate variables $h_l$ are extended to include a constant scalar 1 in $h_l$, so that a linear layer can simply be expressed as $W_l h_l$. The last layer’s output $h_L$ with dimensionality $n_L$ specifies the natural parameter of the exponential family.

We need the following Lemma which gives the FIM w.r.t. $h_L$, which is a $n_L \times n_L$ matrix in simple closed form for commonly used probability distributions.

**Lemma 2.** For the neural network model specified in Eq. (3),

$$\mathcal{I}(h_L) = \text{Cov}(t(y)) = \frac{\partial \eta}{\partial h_L},$$

where $\text{Cov}(\cdot)$ denotes the covariance matrix w.r.t. $p(y \mid x, \theta)$, $\eta := \eta(h_L) := \partial F / \partial h_L$ is the expectation parameters, and the vector-vector-derivative $\partial \eta / \partial h_L$ denotes the Jacobian matrix of the mapping $h_L \rightarrow \eta$.

The derivatives of the log-likelihood $\ell(\theta) := \log p(x, y \mid \theta)$ characterize its landscape and are essential to compute the FIM. By Eq. (3), the score function (gradient of $\ell$) is

$$\frac{\partial \ell}{\partial \theta} = \left( \frac{\partial h_L}{\partial \theta} \right)^\top (t(y) - \eta(h_L)) = \frac{\partial h_L^\top}{\partial \theta} (t_a - \eta_a).$$ (4)

In this paper, we mix the usual $\Sigma$-notation of summation with the Einstein notation: in the same term, an index appearing in both upper- and lower-positions indicates a sum over this index. For example, $t_a h^a = \sum_a t_a h_a$. Hence, in our equations, upper- and lower-indexes have the same meaning: both $h^a$ and $h_a$ mean the $a$'th element of $h$. For convenience and consistency, we take quantities w.r.t. $\theta$ as upper indexed and other quantities as lower indexed, i.e., $\mathcal{I}^{ij}(\theta)$ versus $\mathcal{I}_{ij}(h_L)$. This mixed representation of sums helps to simplify our expressions without causing confusion. From Eq. (4) and Lemma 2, the Hessian of $\ell$ is given by

$$\frac{\partial^2 \ell}{\partial \theta \partial \theta^\top} = (t_a - \eta_a) \frac{\partial^2 h_L^a}{\partial \theta \partial \theta^\top} - \frac{\partial h_L^a}{\partial \theta} \frac{\partial \eta_a}{\partial \theta} = (t_a - \eta_a) \frac{\partial^2 h_L^a}{\partial \theta \partial \theta^\top} - \frac{\partial h_L^a}{\partial \theta} \mathcal{I}_{a \theta}(h_L) \frac{\partial h_L^\theta}{\partial \theta^\top}. $$ (5)
Similar to the case of a general statistical model, the FIM is equivalent to the expectation of the Hessian of $-\ell$ as long as the activation function is smooth enough.

**Theorem 3.** Consider the neural network model in Eq. (3). For any activation function $\sigma \in C^2(\mathcal{H})$ (both $\sigma'(z)$ and $\sigma''(z)$ exist and are continuous), we have $\mathcal{I}(\theta) = \mathbb{E}_p \left( -\frac{\partial^2 \ell}{\partial \theta \partial \theta^\top} \right)$.

**Remark 3.1.** ReLU networks do not have this equivalent expression as ReLU$(z)$ is not differentiable at $z = 0$.

Through the definition of the FIM, or alternatively its equivalent formula in Theorem 3, we arrive at the same expression

$$\mathcal{I}(\theta) = \left( \frac{\partial h_L}{\partial \theta} \right) \mathcal{I}(h_L) \frac{\partial h_L}{\partial \theta} = \frac{\partial h_L^2}{\partial \theta} \mathcal{I}_{ab}(h_L) \frac{\partial h_L}{\partial \theta}^\top.$$ (6)

Equation (6) takes the form of a generalized Gauss-Newton matrix [Martens, 2020]. This general expression of the FIM has been known in the literature [Park et al., 2000, Pascanu and Bengio, 2014]. Under weak conditions, $\mathcal{I}(\theta)$ is a pullback metric [Sun, 2020] of $\mathcal{I}(h_L)$ in Lemma 2 associated with the mapping $\theta \rightarrow h_L$. To compute $\mathcal{I}(\theta)$ in closed form, one need first to compute the Jacobian matrix of size $n_L \times \dim(\theta)$ then perform the matrix multiplication in Eq. (6). The naive algorithm to evaluate Eq. (6) has a computational complexity of $O(n_L^2 \dim(\theta) + n_L \dim^2(\theta))$, where the term $O(n_L \dim^2(\theta))$ is dominant as $\dim(\theta) \gg n_L$ in deep architectures. Once the parameter $\theta$ is updated, the FIM has to be recomputed. This is infeasible in practice for large networks where $\dim(\theta)$ can be millions or billions.

The two estimators $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ in Eq. (2) provide a computationally inexpensive way to estimate the FIM. Given $\theta$ and $x$, one can draw i.i.d. samples $y_1, \ldots, y_N \sim p(y \mid x, \theta)$. Both $\partial \ell_i / \partial \theta$ and $\partial^2 \ell_i / \partial \theta \partial \theta^\top$ can be evaluated directly through auto-differentiation (AD) that is highly optimized for modern GPUs. For $\hat{\mathcal{I}}_1(\theta)$, we already have $\partial \ell_i / \partial \theta$ to perform gradient descent. For $\hat{\mathcal{I}}_2(\theta)$, efficient methods to compute the Hessian are implemented in AD frameworks such as PyTorch [Paszke et al., 2019]. Using these derivatives, the computational cost only scales with the number $N$ of samples but does not scale with $n_L$.

We rarely need the full FIM of size $\dim(\theta) \times \dim(\theta)$. Most of the time, only its diagonal blocks are needed, where each block corresponds to a subset of parameters, e.g., the neural network weights of a particular layer. Therefore the computation of both estimators can be further reduced.

If $p(y \mid x, \theta)$ has the parametric form in Eq. (3), from Eqs. (4) and (5), the FIM estimators become

$$\hat{\mathcal{I}}_1(\theta) = \frac{\partial h_L^2}{\partial \theta} - \frac{1}{N} \sum_{i=1}^{N} (t_a(y_i) - \eta_a)(t_b(y_i) - \eta_b) \cdot \frac{\partial h_L^2}{\partial \theta^\top},$$ (7)

$$\hat{\mathcal{I}}_2(\theta) = \left( \eta_a - \frac{1}{N} \sum_{i=1}^{N} t_a(y_i) \right) \frac{\partial^2 h_L^2}{\partial \theta \partial \theta^\top} + \frac{\partial h_L^2}{\partial \theta} \mathcal{I}_{ab}(h_L) \frac{\partial h_L}{\partial \theta}^\top.$$ (8)

Recall that the notation of $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ is abused as they depend on $x$ and $y_i \cdots y_N$. Notably, in Eq. (7), $\hat{\mathcal{I}}_1(\theta)$ is expressed in terms of the Jacobian matrix of the mapping $\theta \rightarrow h_L$ and the empirical variance of the minimal sufficient statistic $t(y_i)$ of the output exponential family. In Eq. (8), $\hat{\mathcal{I}}_2(\theta)$ depends on both the Jacobian and Hessian of $\theta \rightarrow h_L$ and the empirical average of $t(y_i)$. The second term on the right-hand side (RHS) of Eq. (8) is exactly the FIM, and therefore the first term serves as a bias term. Eqs. (7) and (8) are only for the case with exponential family output. If the output units belong to non-exponential families, e.g., a statistical mixture model, one falls back to the general formulae, i.e., Eq. (2) for the FIM.

As an application of the Fisher information, the Cramér-Rao lower bound (CRLB) states that any unbiased estimator $\hat{\theta}$ of the parameters $\theta$ satisfies $\text{Cov}(\hat{\theta}) \geq \left[ \mathcal{I}(\theta) \right]^{-1}$. For example, in Lemma 2, the FIM...
is w.r.t. the output of the neural network. As such, \( \mathcal{I}(h_L) \) can be used to study the estimation covariance of \( h_L \) based on random samples \( y_1 \cdots y_N \) drawn from \( p(y \mid x, \theta) \). Similarly for Eq. (6), we can consider unbiased estimators of the weights of the neural network. In any case, to apply the CRLB, one needs an accurate estimation of \( \mathcal{I}(\theta) \). If the scale of \( \mathcal{I}(\theta) \) is relatively small when compared to its covariance, its estimation \( \hat{\mathcal{I}}(\theta) \) is more likely to be a small positive value (or even worse, zero or negative). The empirical computation of the CRLB is not meaningful in this case.

3 The Variance of the FIM Estimators

Based on the deep learning architecture specified in Eq. (3), we measure the quality of the two estimators \( \hat{\mathcal{I}}_1(\theta) \) and \( \hat{\mathcal{I}}_2(\theta) \) given by their variances. Given the same sample size \( N \), a smaller variance is preferred as the estimator is more accurate and likely to be closer to the true FIM \( \mathcal{I}(\theta) \). We study how the structure of the exponential family has an impact on the variance.

3.1 Variance in closed form

We first consider \( \hat{\mathcal{I}}_1(\theta) \) and \( \hat{\mathcal{I}}_2(\theta) \) in Eq. (2) as real matrices of dimension \( \dim(\theta) \times \dim(\theta) \). As \( \hat{\mathcal{I}}_1(\theta) \) is a square matrix, the corresponding covariance is a 4D tensor \( \left[ \text{Cov} \left( \hat{\mathcal{I}}_1(\theta) \right) \right]^{ijkl} \) of dimension \( \dim(\theta) \times \dim(\theta) \times \dim(\theta) \times \dim(\theta) \), representing the covariance between the two elements \( \hat{\mathcal{I}}_1^{ij}(\theta) \) and \( \hat{\mathcal{I}}_1^{kl}(\theta) \). The element-wise variance of \( \hat{\mathcal{I}}_1(\theta) \) is a matrix with the same size of \( \hat{\mathcal{I}}_1(\theta) \), which we denote as \( \text{Var}(\hat{\mathcal{I}}_1(\theta)) \). Thus,

\[
\text{Var}(\hat{\mathcal{I}}_1(\theta))^{ij} = \left[ \text{Cov} \left( \hat{\mathcal{I}}_1(\theta) \right) \right]^{ijij}.
\]

Similarly, the covariance and element-wise variance of \( \hat{\mathcal{I}}_2(\theta) \) are denoted as \( \left[ \text{Cov} \left( \hat{\mathcal{I}}_2(\theta) \right) \right]^{ijkl} \) and \( \text{Var}(\hat{\mathcal{I}}_2(\theta))^{ij} \), respectively.

As the samples \( y_1, \ldots, y_N \) are i.i.d., we have

\[
\text{Cov}(\hat{\mathcal{I}}_1(\theta)) = \frac{1}{N} \text{Cov} \left( \frac{\partial \ell}{\partial \theta}, \frac{\partial \ell}{\partial \theta} \right) \quad \text{and} \quad \text{Cov}(\hat{\mathcal{I}}_2(\theta)) = \frac{1}{N} \text{Cov} \left( \frac{\partial^2 \ell}{\partial \theta \partial \theta^t} \right).
\]

Both \( \text{Cov}(\hat{\mathcal{I}}_1(\theta)) \) and \( \text{Cov}(\hat{\mathcal{I}}_2(\theta)) \) have an order of \( O(1/N) \). For the neural network model in Eq. (3), we further have those covariance tensors in closed form.

Theorem 4.

\[
\left[ \text{Cov} \left( \hat{\mathcal{I}}_1(\theta) \right) \right]^{ijkl} = \frac{1}{N} \text{Cov} \left( \frac{\partial \ell}{\partial \theta}, \frac{\partial \ell}{\partial \theta}, \frac{\partial \ell}{\partial \theta}, \frac{\partial \ell}{\partial \theta} \right)
\]

\[
= \frac{1}{N} \partial_i h_L^a(x) \partial_j h_L^b(x) \partial_k h_L^c(x) \partial_l h_L^d(x) \cdot (K_{abcd}(t) - \mathcal{I}_{ab}(h_L) \cdot \mathcal{I}_{cd}(h_L)),
\]

where the 4D tensor

\[
K_{abcd}(t) := \mathbb{E} \left[ (t_a - \eta_a(h_L(x)))(t_b - \eta_b(h_L(x)))(t_c - \eta_c(h_L(x)))(t_d - \eta_d(h_L(x))) \right]
\]

is the 4th (unscaled) central moment\(^1\) of \( t(y) \) and \( \partial_i h_L(x) := \partial_i h_L(x)/\partial \theta_i \).

\(^1\)The kurtosis of a random variable is defined by its 4th standardized (both centered and normalized) moment. Here, \( K(\cdot) \) denotes the 4th central moment but not the kurtosis.
Remark 4.1. The 4D tensor \((\mathcal{K}_{abcd}(t) - \mathcal{I}_{ab}(h_L) \cdot \mathcal{I}_{cd}(h_L))\) is the covariance of the random matrix

\[
\frac{\partial \ell}{\partial \theta_L} \cdot \frac{\partial \ell}{\partial \theta_L^\top} = (t(y) - \eta)(t(y) - \eta)^\top,
\]

where \(y \sim p(y | h_L)\). This random matrix is an estimator of \(\mathcal{I}(h_L)\), i.e. the FIM w.r.t. the natural parameters \(h_L\). Theorem 4 describes how the covariance tensor adapts w.r.t. the coordinate transformation \(h_L \rightarrow \theta\).

Notably, as \(t(y)\) is the sufficient statistics of an exponential family, the derivatives of the log-partition function \(F(h)\) w.r.t. the natural parameters \(h\) are equivalent to the cumulants of \(t(y)\). The cumulants correspond to the coefficients of the Taylor expansion of the logarithm of the moment generating function [McCullagh, 2018]. Importantly, the cumulants of order 3 and below are equivalent to the central moments (see e.g. Lemma 2). However, this is not the case for the 4th central moment which must be expressed as a combination of the 2nd and 4th cumulants, as stated in the following Lemma.

Lemma 5.

\[
\mathcal{K}_{abcd}(t) = \kappa_{abcd} + \mathcal{I}_{ab}(h_L) \cdot \mathcal{I}_{cd}(h_L) + \mathcal{I}_{ac}(h_L) \cdot \mathcal{I}_{bd}(h_L) + \mathcal{I}_{ad}(h_L) \cdot \mathcal{I}_{bc}(h_L),
\]

where

\[
\kappa_{abcd} := \frac{\partial^4 F(h)}{\partial h_a \partial h_b \partial h_c \partial h_d} \big|_{h=h_L(x)}.
\]

Remark 5.1. In the 1D case, the 4th central moment simplifies to \(\mathcal{K}(t) = F''''(h_L) + 3(F''(h_L))^2\).

For the second estimator \(\hat{\mathcal{I}}_2(\theta)\), the covariance only depends on the 2nd central moment of \(t(y)\).

Theorem 6.

\[
\text{Cov} \left( \hat{\mathcal{I}}_2(\theta) \right)_{ijkl} = \frac{1}{N} \cdot \text{Cov} \left( - \frac{\partial^2 \ell}{\partial \theta_i \partial \theta_j} - \frac{\partial^2 \ell}{\partial \theta_i \partial \theta_j} \right) = \frac{1}{N} \cdot \partial^2_{ij} h_L^2(x) \partial^2_{ij} h_L^2(x) \mathcal{I}_{\alpha \beta}(h_L),
\]

where \(\partial^2_{ij} h_L(x) := \frac{\partial^2 h_L(x)}{\partial \theta_i \partial \theta_j}\).

Remark 6.1. By Lemma 2, the matrix \(\mathcal{I}_{\alpha \beta}(h_L)\) is the covariance of the sufficient statistic \(t(y)\). Hence, the covariance of \(\hat{\mathcal{I}}_2(\theta)\) scales with the covariance of \(t(y)\). If \(t(y)\) tends to be deterministic, then the covariance of \(\hat{\mathcal{I}}_2(\theta)\) shrinks towards 0 and its estimation of the FIM becomes accurate.

The covariance in Theorems 4 and 6 has two different components: ① the derivatives of the deep neural network; and ② the central (unscaled) moments of \(t(y)\). The 4D tensor \(\mathcal{K}_{abcd}(t)\) and the 2D FIM \(\mathcal{I}_{\alpha \beta}(h_L)\) correspond to the 4th and 2nd central moments of \(t(y)\), respectively. Intuitively, the larger the scale of the Jacobian or the Hessian of the neural network mapping \(\theta \rightarrow h_L\) and/or the larger the central moments of the exponential family, the lower the accuracy when estimating the FIM.

Additionally, in Appendix C we show that under reparametrization of the neural network weights \(\hat{\mathcal{I}}_1(\theta)\) is a covariant tensor, just like the FIM. Contrarily, \(\hat{\mathcal{I}}_2(\theta)\) does not have this property.

3.2 Variance Bounds

We aim to derive meaningful upper bounds of the covariances presented in Theorems 4 and 6. Using the Cauchy-Schwarz inequality, we can “decouple” the derivatives of the neural network mapping and the central moments of the exponential family into different terms. This provides various bounds on the scale of covariance quantities.

\[\text{In this paper, the derivatives are by default taken w.r.t. } \theta. \text{ Therefore, } \partial_i := \frac{\partial}{\partial \theta_i} \text{ and } \partial^2_{ij} := \frac{\partial^2}{\partial \theta_i \partial \theta_j}.\]
Theorem 7.

\[
\| \text{Cov} \left( \hat{I}_1(\theta) \right) \|_F \leq \frac{1}{N} \| \frac{\partial h_L}{\partial \theta} \|_F^4 \cdot \| K(t) - \mathcal{I}(h_L) \otimes \mathcal{I}(h_L) \|_F,
\]

where \( \otimes \) is the tensor-product: \((\mathcal{I}(h_L) \otimes \mathcal{I}(h_L))_{abcd} := \mathcal{I}_{ab}(h_L) \cdot \mathcal{I}_{cd}(h_L)\).

The scale \( \| \text{Cov} \left( \hat{I}_1(\theta) \right) \|_F \) measures how much the estimator \( \hat{I}_1(\theta) \) deviates from \( \mathcal{I}(\theta) \). Theorem 7 says that this deviation is bounded by the scale of the Jacobian matrix \( \frac{\partial h_L}{\partial \theta} \) as well as the scale of \((K(t) - \mathcal{I}(h_L) \otimes \mathcal{I}(h_L))\). Recall from Remark 4.1 the latter measures the variance when estimating the FIM \( \mathcal{I}(h_L) \) of the exponential family. Theorem 7 allows us to study these two different factors separately.

Theorem 8.

\[
\| \text{Cov} \left( \hat{I}_2(\theta) \right) \|_F \leq \frac{1}{N} \| \frac{\partial^2 h_L(x)}{\partial \theta \partial \theta^T} \|_F^2 \cdot \| \mathcal{I}(h_L) \|_F.
\]

On the RHS, the Hessian \( \frac{\partial^2 h_L(x)}{\partial \theta \partial \theta^T} \) is a 3D tensor of shape \( n_L \times \text{dim}(\theta) \times \text{dim}(\theta) \). Therefore, the variance of \( \hat{I}_2(\theta) \) is bounded by the scale of the Hessian, as well as the scale of the FIM \( \mathcal{I}(h_L) \) of the output exponential family.

We consider an upper bound to further simplify related terms in Theorems 7 and 8.

Lemma 9.

\[
\| K(t) - \mathcal{I}(h_L) \otimes \mathcal{I}(h_L) \|_F \leq \sqrt{2} \left( \sum_{a=1}^{n_L} \left( \sqrt{K_{aaaa}(t)} + \mathcal{I}_{aa}(h_L) \right) \right)^2,
\]

\[
\| \mathcal{I}(h_L) \|_F \leq \sum_{a=1}^{n_L} \mathcal{I}_{aa}(h_L).
\]

Remark 9.1. Using Lemma 9, it is straightforward to bound the scale of the covariance tensors with the size of the Jacobian/Hessian, as well as the central moments \( K_{aaaa}(t) \) and \( \mathcal{I}_{aa}(h_L) \). These bounds are meaningful but omitted for brevity.

Remark 9.2. By Lemma 9, \( \| K(t) - \mathcal{I}(h_L) \otimes \mathcal{I}(h_L) \|_F \) is in the order of \( O(n_L^2) \) and \( \| \mathcal{I}(h_L) \|_F \) is in the order of \( O(n_L) \).

The scale of the tensors \( K(t) - \mathcal{I}(h_L) \otimes \mathcal{I}(h_L) \) and \( \mathcal{I}(h_L) \) is bounded by the diagonal elements of \( K(t) \) and \( \mathcal{I}(h_L) \), or the element-wise central moments of \( t(y) \). Understanding the scale of these 1D central moments helps to understand the scale of the moment terms in our key statements.

Table 1 presents some 1D exponential families and their cumulants. Figure 1 displays \( K(t) - \text{Var}^2(t) \) and \( \text{Var}(t) \) against the mean of these distributions. Based on Fig. 1a, if the neural network has Bernoulli output units, then the scale of \( K_{aaaa}(t) - (\mathcal{I}_{aa}(h_L))^2 \) is smaller than \( \mathcal{I}_{aa}(h_L) \) regardless of \( h_L \). Notably, when \( p = 0.5 \), the variance of the first estimator \( \hat{I}_1(\theta) \) is 0 --- regardless of \( h_L \). For normal distribution output units (corresponding to the mean squared error loss) in Fig. 1b, both central moment quantities are constant. For Poisson output units in Fig. 1c, \( \mathcal{I}_{aa}(h_L) \) increases linearly with the average number of events \( \lambda \), while \( K_{aaaa}(t) - (\mathcal{I}_{aa}(h_L))^2 \) increases quadratically. Thus, the upper bound of \( \| \text{Cov}(\hat{I}_2(\theta)) \|_F \) increases faster than the upper bound of \( \| \text{Cov}(\hat{I}_2(\theta)) \|_F \) as \( h_L \) enlarges. In this case, one may prefer \( \hat{I}_2(\theta) \) rather than \( \hat{I}_1(\theta) \) and/or control the scale of \( h_L \). In general, \( h_L \) is desired to be in certain regions in the parameter space of the exponential family to control the estimation variance of the FIM. Techniques
Table 1: Cumulants of univariate exponential family distributions, given by derivatives of the log-partition function. \( p, \mu \) and \( \lambda \) denote the mean of the Bernoulli, normal, and Poisson distributions, respectively. † The normal distribution has unit standard deviation \( (\sigma = 1) \).

| DIST. | \( F(h) \) | \( h \) | \( \partial^2 F(h) \) | \( \partial^4 F(h) \) |
|-------|-------------|--------|----------------|------------------|
| BERNOULLI | \( \log(1 + \exp(h)) \) | \( \log p/1-p \) | \( p(1-p) \) | \( p(1-p)(6p^2 - 6p + 1) \) |
| NORMAL† | \( h^2/2 \) | \( \mu \) | \( 1 \) | \( 0 \) |
| POISSON | \( \exp(h) \) | \( \log \lambda \) | \( \lambda \) | \( \lambda \) |

(a) Bernoulli. (b) Normal \( (\sigma = 1) \). (c) Poisson.

Figure 1: The scale of \( K(t) - \text{Var}^2(t) \) and \( \text{Var}(t) \) for the exponential family distributions in Table 1.

to achieve this include regularization on the scale of \( h_L \); temperature scaling [Hinton et al., 2015]; or normalization layers [Ba et al., 2016, Salimans and Kingma, 2016]. Of course, they could inversely increase the scale of the derivatives of the neural network, which can be controlled by imposing additional constraints, i.e., Lipschitz requirements.

See Appendix G for numerical verifications of the bounds in Theorems 7 and 8 on the MNIST dataset.

3.3 Positive Definiteness

By definition, the FIM of any statistical model is positive semidefinite (p.s.d.). The first estimator \( \hat{I}_1(\theta) \) is naturally on the p.s.d. manifold (space of p.s.d. matrices). On the other hand, \( \hat{I}_2(\theta) \) can “fall off” the p.s.d. manifold. It is important to examine the likelihood for \( \hat{I}_2(\theta) \) having a negative spectrum and the corresponding scale, so that any algorithm (e.g., natural gradient) relying on the FIM being p.s.d. can be adapted.

Eq. (8) can be re-expressed as the sum of a p.s.d. matrix and a linear combination of \( n_L \) symmetric matrices. We provide the likelihood for \( \hat{I}_2(\theta) \) staying on the p.s.d. manifold given conditions on the spectrum of the Hessian.

**Theorem 10.** Let \( \lambda_{\min}(\cdot), \lambda_{\max}(\cdot), \) and \( \rho(\cdot) \) denote the smallest eigenvalue, the largest eigenvalue, and the spectral radius (largest absolute value of the spectrum), respectively. Let \( \rho := (\rho(\partial^2 h_L^1), \cdots, \rho(\partial^2 h_L^{n_L})) \). If \( \lambda_{\min}(I(\theta)) > 0 \), then with probability at least

\[
1 - \frac{n_L \cdot \|\rho\|^2 \cdot \lambda_{\max}(I(h_L))}{N \cdot \lambda_{\min}^2(I(\theta))},
\]

the estimator \( \hat{I}_2(\theta) \) with \( N \) samples is a p.s.d. matrix.

The bound becomes uninformative as the output layer size \( n_L \) increases, as the spectrum of the Hessian of \( h_L \) scales up, or as the spectrum of the FIM \( I(h_L) \) enlarges. On the other hand, as the minimal
eigenvalue of the FIM $\mathcal{I}(\theta)$ increases, Theorem 10 can give meaningful lower bounds. In particular, with sample rate $O(N^{-1})$, estimator $\hat{\mathcal{I}}_2(\theta)$ will be a p.s.d. matrix. In practice for over-parametrized networks, $\lambda_{\min}(\mathcal{I}(\theta))$ is close to or equals 0 and Theorem 10 is not meaningful. In any case, we need to consider the scale of the negative spectrum of $\hat{\mathcal{I}}_2(\theta)$.

**Theorem 11.**

$$\lambda_{\min}(\hat{\mathcal{I}}_2(\theta)) \geq -\rho(\partial^2 h_L^a(x)) \left\| \eta_a - \frac{1}{N} \sum_{i=1}^{N} t_a(y_i) \right\|.$$ 

Theorem 11 guarantees that in the worst case, the scale of the negative spectrum of $\hat{\mathcal{I}}_2(\theta)$ is controlled. By Lemma 2, $\text{Var}(\eta_a - \frac{1}{N} \sum_{i=1}^{N} t_a(y_i)) = \frac{1}{N} \mathcal{I}^{aa}(h_L)$. Therefore, as $N$ increases or $\mathcal{I}^{aa}(h_L)$ decreases, the negative spectrum of $\hat{\mathcal{I}}_2(\theta)$ will shrink. Further analysis on the spectrum of $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ can utilize the geometric structure of the p.s.d. manifold. This is left for future work.

### 3.4 Convergence Rate

The rate of convergence for each of the estimators is of particular interest when considering their practical viability. Through a generalized Chebyshev inequality [Chen, 2007], we can get a simple Frobenius norm convergence rate.

**Lemma 12.** Let $0 < \varepsilon < 1$. Then

$$\left\| \hat{\mathcal{I}}_1(\theta) - \mathcal{I}(\theta) \right\|_F \leq \frac{1}{\sqrt{\varepsilon N}} \sqrt{\sum_{i,j=1}^{\dim(\theta)} \text{Var} \left( \frac{\partial \ell}{\partial \theta_i} \frac{\partial \ell}{\partial \theta_j} \right)},$$

holds with probability at least $1 - \varepsilon$; and

$$\left\| \hat{\mathcal{I}}_2(\theta) - \mathcal{I}(\theta) \right\|_F \leq \frac{1}{\sqrt{\varepsilon N}} \sqrt{\sum_{i,j=1}^{\dim(\theta)} \text{Var} \left( -\frac{\partial^2 \ell}{\partial \theta_i \partial \theta_j} \right)},$$

hold with probability at least $1 - \varepsilon$.

Each of these convergence rates only depends on the element-wise variance of the estimator terms in Eq. (9). Moreover, each of the estimators has a convergence rate of $O(N^{-1/2})$. The rate’s constants are determined by the variance of the estimators given by Theorems 4 and 6, which are influenced by the derivatives of the neural network and the moments of the output exponential family.

### 4 Effect of Neural Network Derivatives

The derivatives of the deep learning network can affect the estimation variance of the FIM. By Theorem 4, the variance of the first estimator $\hat{\mathcal{I}}_1(\theta)$ scales with the Jacobian of the neural network mapping $\theta \rightarrow h_L(x)$. By Theorem 6, the variance of $\hat{\mathcal{I}}_2(\theta)$ scales with the Hessian of $\theta \rightarrow h_L(x)$. The larger the scale of the Jacobian or the Hessian, the larger the estimation variance. In this section, we examine these derivatives in more detail.

We give the closed form gradient of the log-likelihood $\ell$ and the last layer’s output $h_L$ w.r.t. the neural network parameters.
Lemma 13.
\[
\frac{\partial \ell}{\partial W_l} = D_l \frac{\partial \ell}{\partial h_{l+1}} \bar{h}_l^\top, \quad \frac{\partial \ell}{\partial h_l} = B_l^\top (t(y) - \eta(h_L)), \quad \frac{\partial h_l}{\partial W_l} = D_l B_l^\top e_a \bar{h}_l^\top,
\]
where \(e_a\) is the \(a\)th standard basis vector, \(B_l\) and \(D_l\) are recursively defined by
\[
B_L = I, \quad B_l = B_{l+1} D_l W_l^{-}, \\
D_{L-1} = I, \quad D_l = \text{diag}(\sigma'(W_l h_l)),
\]
\(I\) is the identity matrix, and \(\text{diag}(\cdot)\) means a diagonal matrix with given diagonal entries.

By Lemma 13, we can estimate the FIM w.r.t. the hidden representations \(h_l\) through
\[
\hat{I}_l(h_l) = \frac{1}{N} \sum_{i=1}^N \frac{\partial \ell}{\partial h_i} \frac{\partial \ell}{\partial h_i^\top} = B_l^\top \left( \frac{1}{N} \sum_{i=1}^N (t(y_i) - \eta(h_L)) (t(y_i) - \eta(h_L))^\top \right) B_l.
\]

As \(B_l\) is recursively evaluated from the last layer to previous layers, the FIM can also be recursively estimated based on \(\hat{I}_l(\theta)\). It is similar to back-propagation, except that the FIMs are back-propagated instead of gradients of the network. This is similar to the backpropagated metric [Ollivier, 2015].

To investigate how the first estimator \(\hat{I}_l(\theta)\) is affected by the loss landscape, we bound the Frobenius norm of the parameter-output Jacobian \(\partial h_L / \partial \theta\).

Lemma 14. If the activation function has bounded gradient and \(\forall z \in \mathbb{R}, |\sigma'(z)| \leq 1\), then
\[
\sum_{i=1}^L \left\| \frac{\partial h_L}{\partial W_i} \right\|_F \leq \prod_{i=l+1}^L \left\| W_i^{-} \right\|_F \left\| \bar{h}_l \right\|_2,
\]

where \(\frac{\partial h_L}{\partial W_i} = [\partial h_1^L / \partial W_i, \ldots, \partial h_L^L / \partial W_i]\) is the derivative of a vector w.r.t. a matrix that is a 3D tensor.

Given Lemma 14, we see that the gradient \(\partial h_L / \partial W_i\) scales with both the neural network weights \(W_i\) and the gradient of the activation function \(D_l\). Common activation functions have both bounded outputs and 1st-order derivatives; or at least are locally Lipschitz, i.e., sigmoid and ReLU activation functions. During training, regularizing the scale of the neural network weights is a sufficient condition for bounding the variance of \(\hat{I}_l(\theta)\).

An alternative bound can be established which depends on the maximum singular values of the weight matrices.

Lemma 15. Suppose that the activation function has bounded gradient \(\forall z \in \mathbb{R}, |\sigma'(z)| \leq 1\). Then
\[
\sum_{i=1}^L \left\| \frac{\partial h_L}{\partial W_i} \right\|_{2,\sigma} \leq \left( \prod_{i=l+1}^L s_{\text{max}}(W_i^{-}) \right) \left\| \bar{h}_l \right\|_2,
\]

where \(s_{\text{max}}(\cdot)\) denotes the maximum singular value and \(\left\| T \right\|_{2,\sigma}\) denotes the tensor spectral norm for a 3D tensor \(T\), defined by
\[
\left\| T \right\|_{2,\sigma} = \max \{ \langle T, \alpha \otimes \beta \otimes \gamma \rangle : \left\| \alpha \right\|_2 = \left\| \beta \right\|_2 = \left\| \gamma \right\|_2 = 1 \}.
\]

Therefore, regularizing \(s_{\text{max}}(W_i^{-})\), or the spectral norm of the weight matrices, also helps to improve the estimation accuracy of the FIM.
We further reveal the relationship between the loss landscape and the FIM estimators. For a given target \( \hat{y} \), the log-likelihood is denoted as \( l := \log p(\hat{y} \mid x, \theta) \). Furthermore, let us define \( \Delta \hat{I}_1(\theta) := (\partial \hat{l}/\partial \theta)(\partial \hat{l}/\partial \theta^\top) - \hat{I}_1(\theta) \) and \( \Delta \hat{I}_2(\theta) := -\partial^2 \hat{l}/\partial \theta \partial \theta^\top - \hat{I}_2(\theta) \). By Eqs. (4) and (5),

\[
\Delta \hat{I}_1(\theta) = \frac{\partial h_b^a}{\partial \theta} \left( t_a(\hat{y}) - \eta_a(t_b(\hat{y}) - \eta_b) - \frac{1}{N} \sum_{i=1}^N (t_a(y_i) - \eta_a)(t_b(y_i) - \eta_b) \right) \frac{\partial h_b^a}{\partial \theta^\top},
\]

\[
\Delta \hat{I}_2(\theta) = \left[ \frac{1}{N} \sum_{i=1}^N t_a(y_i) - t_a(\hat{y}) \right] \frac{\partial^2 h_b^a}{\partial \theta \partial \theta^\top}.
\]

Hence, the difference between \( \tilde{I}_1(\theta) \) (resp. \( \tilde{I}_2(\theta) \)) and the squared gradient (resp. Hessian) of the loss \(-\hat{\ell}\) depends on how \( y \) differs from \( \hat{y} \). If the network \( \theta \) is trained, then the random samples \( y_i \sim p(y \mid x, \theta) \) are close to the given target \( \hat{y} \). In this case, \( \tilde{I}_1(\theta) \) corresponds to the squared gradient, and \( \tilde{I}_2(\theta) \) corresponds to the Hessian. This is not true for untrained neural networks with random weights.

5 Related Work

The two estimators \( \tilde{I}_1(\theta) \) and \( \tilde{I}_2(\theta) \) are not new as one usually utilizes one of them to compute the FIM. Guo and Spall [2019] analyzed their accuracy for univariate symmetric density functions based on the central limit theorem. Fisher information estimation is also examined in latent variable models [Delattre and Kuhn, 2019]. Under the same topic, our work analyzes the factors affecting the variance of \( \tilde{I}_1(\theta) \) and \( \tilde{I}_2(\theta) \) for deep neural networks.

A large body of work tries to approximate the FIM or define similar curvature tensors for performing natural gradient descent [Amari, 2016, Martens, 2020, Martens and Grosse, 2015, Kingma and Ba, 2015, Ollivier, 2015, Sun and Nielsen, 2017]. If the loss is an empirical expectation of \(-\log p(y \mid x, \theta)\), its Hessian w.r.t. \( h_{Li} \) is exactly \( I(h_{Li}) \). Then, the FIM in Eq. (6) is in the form of a Generalized Gauss-Newton matrix (GNN) [Schraudolph, 2002, Martens, 2020, Ollivier [2015] provided algorithm procedures to compute the unit-wise FIM and discussed Monte Carlo natural gradient. The FIM can be computed locally [Sun and Nielsen, 2017, Ay, 2020] based on a joint distribution representation of the neural network. Efficient computational methods are developed to evaluate the FIM inverse [Park et al., 2000].

The estimator \( \tilde{I}_1(\theta) \) is not the “empirical Fisher” (see e.g. [Martens, 2020, Section 11]) as \( y_i \) is randomly sampled from \( p(y \mid x, \theta) \), making \( \tilde{I}_1(\theta) \) an unbiased estimator. The difference between the empirical Fisher and the FIM is clarified [Kunstner et al., 2020]. Similarly, the estimator \( \tilde{I}_2(\theta) \) is not the Hessian of the loss, as \( y_i \) is randomly sampled rather than fixed to the target.

Recently, the structure of the FIM (or its partial approximations) are examined in deep learning. The FIM of randomized networks is analyzed [Amari et al., 2019], where the weights of the neural network are assumed to be random. Often the analysis of randomized networks uses spectral analysis and random matrix theory [Pennington and Worah, 2018]. An insight from this body of work is that most of the eigenvalues of the FIM are close to \( 0 \); while the high end of spectrum has large values [Karakida et al., 2019]. In this paper, the estimators \( \hat{I}_1(\theta) \) and \( \hat{I}_2(\theta) \) are random matrices due to the sampling of \( y_i \sim p(y \mid x) \) (the weights are considered fixed).

In information geometry [Amari, 2016, Nielsen, 2020], the FIM serves as a Riemannian metric in the space of probability distributions. The FIM is a covariant tensor and is invariant to diffeomorphism on the sample space [Nielsen, 2020]. Higher order tensors are used to describe the intrinsic structure in this space. For example, the Riemannian curvature is a 4D tensor, while the Ricci curvature is 2D. The third cumulants of the sufficient statistics give an affine connection (belonging to the \( \alpha \)-connections or the Amari-\v{C}entsov tensor) of the exponential family. The FIM is generalized to a one-parameter family [Nielsen, 2017].

In statistics, our estimator \( \hat{I}_2(\theta) \) is Efron and Hinkley [1978]’s “observed Fisher information”, which is usually evaluated at the maximum likelihood estimation \( \hat{\theta} \). Higher order moments of the maximum
likelihood estimator (MLE) were discussed (see e.g. Bowman and Shenton [1988]). These moments are associated with parameter estimators and differ from the concept of the FIM estimators. Similar concepts are examined in higher-order asymptotic theory [Amari, 2016, Chapter 7].

6 Conclusion

The FIM is a covariant p.s.d. tensor revealing the intrinsic geometric structure of the parameter manifold. It yields useful practical methods such as the natural gradient. In practice, the true FIM $\mathcal{I}(\theta)$ is usually expensive or impossible to obtain. Estimators of the FIM based on empirical samples is used in the deep learning practice. We analyzed two different estimators $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ of the FIM of a deep neural network. These estimators are convenient to compute using auto-differentiation frameworks but randomly deviates from $\mathcal{I}(\theta)$. Our central results, Theorems 4 and 6, present the variance of $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ in closed form, which is further extended to upper bounds in simpler forms. Two factors affecting the estimation variance are

1. the derivatives of neural network output $h_L$ w.r.t. the weight parameters $\theta$; and
2. the property of $h_L$ as an exponential family distribution. A large scale of the 1st- and/or 2nd-order derivatives leads to a large variance when estimating the FIM. Our analytical results can be useful to measure the quality of the estimated FIM and could lead to variance reduction techniques.

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Appendix

This appendix contains a proofs of the results in the main text and further analysis on the two FIM estimators \( \hat{I}_1(\theta) \) and \( \hat{I}_2(\theta) \). In particular, Appendix C presents an analysis of how the FIM estimators and their covariance tensors change under reparametrization. Appendix D presents element-wise bound alternatives to those presented in Section 3.2. Appendix E explores various results using alternative norms to the Frobenius norm results of the main text. Appendix F presents an analysis on taking a linear combination of the two FIM estimators. Appendix G presents a numerical experiments of the FIM estimators on the MNIST dataset.

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A List of Symbols

Table A.2: Table of symbols.

| Symbol | Meaning                                                                 | Defined       |
|--------|-------------------------------------------------------------------------|---------------|
| $\mathcal{I}(\theta)$ | Fisher information matrix (FIM)                                          | Eq. (1)       |
| $\hat{\mathcal{I}}_1(\theta)$ | An estimator of the FIM                                                 | Eq. (2)       |
| $\hat{\mathcal{I}}_2(\theta)$ | Another estimator of the FIM                                             |               |
| $\text{Var}(\cdot)$ | Element-wise variance of input; output is the same dimension as the input dimension | Eq. (9)       |
| $\text{Cov}(\cdot)$ | Pair-wise covariance of input; output is the dimension of an outer product on the input | Lemma 2       |
| $h$ | Natural parameter of exponential family                                  | Table 1       |
| $h_l$ | Hidden layer output in our neural network model                          | Eq. (3)       |
| $h_L$ | Last layer’s output in our neural network model and the natural parameter of the exponential family | Eq. (3)       |
| $n_l$ | Size of layer $l$                                                       | Eq. (3)       |
| $F(h_L)$ | Log-partition function of exponential family                            | Lemma 2       |
| $\eta = \eta(h_L)$ | Dual parameterization of exponential family                             | Lemma 2       |
| $\mathcal{I}(h_L) = \text{Var}(t)$ | Covariance matrix of $t$                                                 | Lemma 2       |
| $K(t)$ | 4th central moment of $t$                                                | Theorem 4     |
| $\kappa_{a,b,c,d}$ | 4th order cumulant of exponential family                                | Lemma 5       |
| $\lambda_{\min}(M)$ | Smallest eigenvalue of $M$                                               | Theorem 10    |
| $\rho(M)$ | Spectral radius of $M$ (absolute value of spectrum)                     | Theorem 10    |
| $\partial \ell / \partial h_L; \partial^2 h_L$ | Partial derivatives of likelihood w.r.t. weights | Eq. (4)       |
| $\|\cdot\|_F$ | Frobenius norm / $L_2$-norm                                              | Proposition 1 |
| $\|\cdot\|_2$ | 2-norm / $L_2$-norm                                                     | Proposition 1 |
| $\|\cdot\|_F$ | Tensor spectral norm                                                    | Lemma 15      |
| $\|\cdot\|_1$ | $L_1$-norm                                                              | Theorem A.6    |
| $\|\cdot\|_\infty$ | $L_\infty$-norm                                                         | Theorem A.6    |
| $M^T$ | Matrix transpose                                                        | Eq. (3)       |
| $\otimes$ | Tensor product                                                          | Lemma A.4     |

B Variance of FIM estimators

B.1 Proof of Proposition 1

Proof. The first statement holds as both $\hat{\mathcal{I}}_1(\theta)$ and $\hat{\mathcal{I}}_2(\theta)$ are point-wise estimators, they are unbiased (central limit theorem).

The second statement holds by the law of large numbers (and triangle inequality with $\epsilon/2$ and a union bound).

B.2 Proof of Lemma 2

Proof. The statement follows as $p(y | x, \theta)$ is given by an exponential family. See Amari [2016].
B.3 Proof of Theorem 3

Proof. Consider the alternative formulation of the FIM.

\[
\mathbb{E}_{x,y} \left[ -\frac{\partial^2}{\partial \theta \partial \theta^\top} \log p(y \mid x) \right] = \mathbb{E}_{x,y} \left[ \frac{\partial \ell}{\partial \theta} \frac{\partial \ell}{\partial \theta^\top} \right] - \mathbb{E}_{x,y} \left[ \frac{\partial^2}{\partial \theta \partial \theta^\top} p(y \mid x) \right]
\]

\[
= I(\theta) - \int p(x) \frac{\partial^2}{\partial \theta \partial \theta^\top} p(y \mid x) \, dy \, dx.
\]

Thus for this to be equivalent to the Jacobian definition, we need the residual term to be zero.

As \( \sigma \in C^2(\mathbb{R}) \) and thus \( \sigma' \) is smooth, it follows by the composition of smooth functions that \( p(y \mid x) \) and \( \partial p(y \mid x) \) is also a smooth function. This provides sufficient conditions for the Leibniz integration rule to be used (switch order of integration and differentiation). As such,

\[
\mathbb{E}_{x,y} \left[ -\frac{\partial^2}{\partial \theta \partial \theta^\top} \log p(y \mid x) \right] = I(\theta) - \int p(x) \frac{\partial^2}{\partial \theta \partial \theta^\top} p(y \mid x) \, dy \, dx
\]

\[
= I(\theta) - \frac{\partial^2}{\partial \theta \partial \theta^\top} \int p(x)p(y \mid x) \, dy \, dx
\]

\[
= I(\theta).
\]

\[
\square
\]

B.4 Proof of Theorem 4

Proof. First define \( \delta := \delta(x, y; \theta) = t(y) - \eta(h_L(x)) \).

\[
\text{Cov} (\partial_\ell \cdot \partial_\ell, \partial_\ell \cdot \partial_\ell) = \mathbb{E}_{y \mid x, \theta} \left[ (\partial_\ell \cdot \partial_\ell) (\partial_\ell \cdot \partial_\ell) \right] - \mathbb{E}_{y \mid x, \theta} [\partial_\ell \cdot \partial_\ell] \cdot \mathbb{E}_{y \mid x, \theta} [\partial_\ell \cdot \partial_\ell].
\]

We then calculate each components. For the first:

\[
\mathbb{E}_{y \mid x, \theta} \left[ (\partial_\ell \cdot \partial_\ell) (\partial_\ell \cdot \partial_\ell) \right] = \mathbb{E}_{y \mid x, \theta} \left[ \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \delta_a \cdot \delta_b \cdot \delta_c \cdot \delta_d \right]
\]

\[
= \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \mathbb{E}_{y \mid x, \theta} [\delta_a \cdot \delta_b \cdot \delta_c \cdot \delta_d].
\]

For the second term, we can first consider the expectation:

\[
\mathbb{E}_{y \mid x, \theta} [\partial_\ell \cdot \partial_\ell]
\]

\[
= \mathbb{E}_{y \mid x, \theta} \left[ \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \delta_a \cdot \delta_b \right]
\]

\[
= \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \mathbb{E}_{y \mid x, \theta} [\delta_a \cdot \delta_b].
\]

Thus the product of this gives:

\[
\mathbb{E}_{y \mid x, \theta} [\partial_\ell \cdot \partial_\ell] \cdot \mathbb{E}_{y \mid x, \theta} [\partial_\ell \cdot \partial_\ell]
\]

\[
= \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \mathbb{E}_{y \mid x, \theta} [\delta_a \cdot \delta_b \cdot \delta_c \cdot \delta_d].
\]

This gives the total covariance:

\[
\text{Cov} (\partial_\ell \cdot \partial_\ell, \partial_\ell \cdot \partial_\ell) = \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \partial_\ell h^2_L(x) \cdot \mathbb{E}_{y \mid x, \theta} [\delta_a \cdot \delta_b \cdot \delta_c \cdot \delta_d].
\]

\[
\square
\]
B.5 Proof of Lemma 5

Proof. We first consider the following notation, consistent with [McCullagh, 2018] except as subscripts, to denote the central moments and different multivariate cumulants. The non-central moment of a vector random variable \(X\) is denoted as
\[
\kappa_{r_1 \ldots r_m} = \mathbb{E}[X_{r_1} \cdots X_{r_m}],
\]
where \(r\) is an integer vector denoting the dimensions in which the non-central moment is taken as. The dimensions can be repeated, i.e., \(r_1 = r_2\) etc. Note that in the notation \(r_1 \ldots r_m\) are not comma separated.

Similarly, for central moments we have:
\[
\mathcal{K}_{r_1 \ldots r_m} = \mathbb{E}[(X_{r_1} - \mathbb{E}[X_{r_1}]) \cdots (X_{r_m} - \mathbb{E}[X_{r_m}])].
\]

For cumulants, we use a comma separated subscripts to distinguish it from central moments. In our case (\(X\) is from an exponential family), this just reduces to \(m\)-derivative of the log-partition function:
\[
\kappa_{r_1,\ldots,r_m} = \frac{\partial^m F(h_L)}{\partial h_{r_1} \cdots \partial h_{r_m}}
\]

In addition to these moment-like quantities, we introduce the \([n]\) notation from [McCullagh, 2018] to denote the possible permutations in indices. For example:
\[
\kappa_i \kappa_{j,k}[3] = \kappa_i \kappa_{j,k} + \kappa_j \kappa_{i,k} + \kappa_k \kappa_{i,j},
\]
noting that the (central and non-central) moments and cumulants are index order invariant. The numbering also must be equal to the number of available permutations. Also note that \(\kappa_i\) denotes a cumulant and not the moment.

[McCullagh, 2018] only provides a formulation from cumulants to non-central moments. Thus we need to rewrite \(K_{abcd}\) in terms of non-central moments. The following is given in [McCullagh, 2018, Equation (2.6)]:
\[
\begin{align*}
\kappa_{ij} &= \kappa_{i,j} + \kappa_i \kappa_j; \\
\kappa_{ijk} &= \kappa_{i,j,k} + \kappa_i \kappa_{j,k} + \kappa_j \kappa_{i,k}; \\
\kappa_{ijkl} &= \kappa_{i,j,k,l} + \kappa_{i,j} \kappa_{k,l} + \kappa_{i,k} \kappa_{j,l} + \kappa_{i,k} \kappa_{l,k}.
\end{align*}
\]

Expanding \(K_{abcd}\), the 4th central moment, yields the following:
\[
\begin{align*}
K_{abcd} &= \kappa_{abcd} - \kappa_a \kappa_{b,c,d}[4] + \kappa_a \kappa_{b,c} \kappa_{e,d}[6] - 3 \kappa_a \kappa_{b,e} \kappa_{c,d} \\
&= \kappa_{abcd} - \kappa_a \kappa_{b,c,d}[4] + (\kappa_a \kappa_{b,c} (\kappa_{e,d} + \kappa_{c,e,d}))[6] - 3 \kappa_a \kappa_{b,c} \kappa_{e,d} \\
&= \kappa_{abcd} - \kappa_a \kappa_{b,c,d}[4] + \kappa_a \kappa_{b,c} \kappa_{e,d}[6] + 3 \kappa_a \kappa_{b,c} \kappa_{e,d} \\
&= \kappa_{abcd} - (\kappa_a (\kappa_{b,c,d} + \kappa_{a,b,c,d}[3] + \kappa_{a,b,c} \kappa_{e,d}))[4] + \kappa_a \kappa_{b,c} \kappa_{e,d}[6] + 3 \kappa_a \kappa_{b,c} \kappa_{e,d} \\
&= \kappa_{abcd} - \kappa_a \kappa_{b,c,d}[4] - \kappa_a \kappa_{b,c} \kappa_{e,d}[6] - \kappa_a \kappa_{b,c} \kappa_{e,d} \\
&= \kappa_{a,b,c,d} [4] + \kappa_{a,b,c,d}[3],
\end{align*}
\]

which when substituting for derivatives proves the Lemma. \(\square\)
B.6 Proof of Theorem 6

Proof.

\[
\text{Cov} \left( -\frac{\partial^2 \ell}{\partial \theta_i \partial \theta_j}, -\frac{\partial^2 \ell}{\partial \theta_k \partial \theta_l} \right) = \text{Cov} \left( \partial_i h^a_L(x) I_{ab}(h_L) \partial_j h^b_L(x) - [t_\alpha(y) - \eta_\alpha] \frac{\partial^2 h^a_L(x)}{\partial \theta_i \partial \theta_j}, \right.
\]

\[
\left. \partial_k h^a_L(x) I_{ab}(h_L) \partial_l h^b_L(x) - [t_\beta(y) - \eta_\beta] \frac{\partial^2 h^a_L(x)}{\partial \theta_k \partial \theta_l} \right).
\]

\[
= \text{Cov} \left( [t_\alpha(y) - \eta_\alpha] \frac{\partial^2 h^a_L(x)}{\partial \theta_i \partial \theta_j}, [t_\beta(y) - \eta_\beta] \frac{\partial^2 h^a_L(x)}{\partial \theta_k \partial \theta_l} \right)
\]

\[
= E \left[ [t_\alpha(y) - \eta_\alpha] \frac{\partial^2 h^a_L(x)}{\partial \theta_i \partial \theta_j} \cdot [t_\beta(y) - \eta_\beta] \frac{\partial^2 h^a_L(x)}{\partial \theta_k \partial \theta_l} \right]
\]

\[
- E \left[ [t_\alpha(y) - \eta_\alpha] \frac{\partial^2 h^a_L(x)}{\partial \theta_i \partial \theta_j} \right] \cdot E \left[ [t_\beta(y) - \eta_\beta] \frac{\partial^2 h^a_L(x)}{\partial \theta_k \partial \theta_l} \right]
\]

\[
= E \left[ [t_\alpha(y) - \eta_\alpha] \frac{\partial^2 h^a_L(x)}{\partial \theta_i \partial \theta_j} \cdot [t_\beta(y) - \eta_\beta] \frac{\partial^2 h^a_L(x)}{\partial \theta_k \partial \theta_l} \right]
\]

\[
= \frac{\partial^2 h^a_L(x)}{\partial \theta_i \partial \theta_j} E[\delta_\alpha \cdot \delta_\beta].
\]

The theorem follows immediately.

\[ \square \]

B.7 Proof of Theorem 7

Proof. Let \(1 \leq p, q \leq \infty\) such that \(1/p + 1/q = 1\). Let \(T_{abcd} = K_{abcd}(t) - I_{ab}(h_L) \cdot I_{cd}(h_L)\). From the last inequality in the proof of Lemma A.4 we have,

\[
\left| \text{Cov} \left( I_{iL}(\theta) \right) \right|_{ijkl} \leq \frac{1}{N} \cdot \|\partial_i h_L(x)\|_p \cdot \|\partial_j h_L(x)\|_p \cdot \|\partial_k h_L(x)\|_p \cdot \|\partial_l h_L(x)\|_p \cdot \|T\|_q.
\]
Thus for the $p$-norm,

$$
\|\text{Cov} \left( \hat{I}_1(\theta) \right) \|_p
= \left( \sum_{i,j,k,l} \left| \text{Cov} \left( \hat{I}_1(\theta) \right) \right|_{ijkl}^p \right)^{1/p}
\leq \frac{1}{N} \cdot \|T\|_q \left( \sum_{i,j} \|\partial_i h_L(x)\|_p \cdot \|\partial_j h_L(x)\|_p \cdot \|\partial_i h_L(x)\|_p \right)^{1/p}
= \frac{1}{N} \cdot \|T\|_q \left( \sum_{i,j} \|\partial_i h_L(x)\|_p \right)^2
= \frac{1}{N} \cdot \|T\|_q \cdot \|\partial h_L(x)\|_p^4.
$$

Thus, by taking the $p = q = 2$ the Theorem holds.

\[\square\]

B.8 Proof of Theorem 8

Proof. Let $1 \leq p, q \leq \infty$ such that $1/p + 1/q = 1$. From the last inequality in the proof of Lemma A.5 we have,

$$
\left| \text{Cov} \left( \hat{I}_2(\theta) \right) \right|_{ijkl} \leq \frac{1}{N} \cdot \|\partial^2_i h_L(x)\|_p \cdot \|\partial^2_j h_L(x)\|_p \cdot \|I(h_L)\|_q
$$

Thus for the $p$-norm,

$$
\|\text{Cov} \left( \hat{I}_2(\theta) \right) \|_q
= \left( \sum_{i,j,k,l} \left| \text{Cov} \left( \hat{I}_2(\theta) \right) \right|_{ijkl}^p \right)^{1/p}
\leq \frac{1}{N} \cdot \|I(h_L)\|_q \cdot \left( \sum_{i,j,k,l} \|\partial^2_i h_L(x)\|_p \cdot \|\partial^2_j h_L(x)\|_p \right)^{1/p}
= \frac{1}{N} \cdot \|I(h_L)\|_q \cdot \left( \sum_{i,j} \|\partial^2_i h_L(x)\|_p \right)^2
= \frac{1}{N} \cdot \|I(h_L)\|_q \cdot \|\partial^2 h_L(x)\|_p^2.
$$

Thus, by taking the $p = q = 2$ the Theorem holds.

\[\square\]
B.9 Proof of Lemma 9

Proof. We first prove the second part of the Lemma, which is simpler.

\[
\|I(h_L)\|_F = \sqrt{\sum_{a,b} \text{Cov}^2(t_a, t_b)}
\]
\[
\leq \sqrt{\sum_{a,b} \text{Var}(t_a) \text{Var}(t_b)} \quad \text{(by Cauchy-Schwarz inequality)}
\]
\[
= \sqrt{\sum_a \text{Var}(t_a) \sum_b \text{Var}(t_b)}
\]
\[
= \sum_a I_{aa}(h_L).
\]

We are left with the first part of the Lemma.

\[
\|K(t) - I(h_L) \otimes I(h_L)\|_F^2
\]
\[
= \sum_{a,b,c,d} \left( \mathbb{E}( (t_a - \eta_a)(t_b - \eta_b)(t_c - \eta_c)(t_d - \eta_d))
\right)^2
\]
\[
\leq 2 \sum_{a,b,c,d} \left( \mathbb{E}^2((t_a - \eta_a)(t_b - \eta_b)) \mathbb{E}^2((t_c - \eta_c)(t_d - \eta_d))
\right)
\]
\[
= 2 \sum_{a,b,c,d} (S_{abcd} + T_{abcd}).
\]

We have

\[
S_{abcd} = \mathbb{E}^2((t_a - \eta_a)(t_b - \eta_b)(t_c - \eta_c)(t_d - \eta_d))
\]
\[
\leq \mathbb{E}((t_a - \eta_a)^2(t_b - \eta_b)^2) \mathbb{E}((t_c - \eta_c)^2(t_d - \eta_d)^2)
\]
\[
\leq \mathbb{E}^{1/2}(t_a - \eta_a)^4 \cdot \mathbb{E}^{1/2}(t_b - \eta_b)^4 \cdot \mathbb{E}^{1/2}(t_c - \eta_c)^4 \cdot \mathbb{E}^{1/2}(t_d - \eta_d)^4
\]
\[
= \sqrt{K_{aaaa}(t)} \cdot \sqrt{K_{bbbb}(t)} \cdot \sqrt{K_{cccc}(t)} \cdot \sqrt{K_{dddd}(t)}.
\]

At the same time,

\[
T_{abcd} = \mathbb{E}^2((t_a - \eta_a)(t_b - \eta_b)(t_c - \eta_c)(t_d - \eta_d))
\]
\[
\leq \mathbb{E}(t_a - \eta_a)^2 \cdot \mathbb{E}(t_b - \eta_b)^2 \cdot \mathbb{E}(t_c - \eta_c)^2 \cdot \mathbb{E}(t_d - \eta_d)^2
\]
\[
= I_{aa}(h_L) \cdot I_{bb}(h_L) \cdot I_{cc}(h_L) \cdot I_{dd}(h_L).
\]
To sum up, we have
\[
\|K(t) - \mathcal{I}(h_L) \otimes \mathcal{I}(h_L)\|_F^2 \leq 2 \sum_{a,b,c,d} (S_{abcd} + T_{abcd})
\]
\[
= 2 \left( \sum_a \sqrt{K_{aaaa}(t)} \right)^4 + 2 \left( \sum_a \mathcal{I}_{aa}(h_L) \right)^4
\]
\[
\leq 2 \left( \sum_a (\sqrt{K_{aaaa}(t)} + \mathcal{I}_{aa}(h_L)) \right)^4.
\]
Taking the square root of both sides gives the result.

\[\square\]

### B.10 Proof of Theorem 10

**Proof.** The estimator is a p.s.d. matrix subtracted by a linear combination of symmetric matrices.

\[
\hat{\mathcal{I}}_2(x; \theta) = \mathcal{I}(\theta) - \frac{1}{N} \sum_{i=1}^N [t(y_i) - \eta(h_L(x))]^\top \frac{\partial^2 h_L(x)}{\partial \theta \partial \theta^\top}
\]

\[
= \mathcal{I}(\theta) - \sum_{a=1}^n (\bar{t}_a - E[\bar{t}_a]) \frac{\partial^2 h_a^2(x)}{\partial \theta \partial \theta^\top},
\]

where \(\bar{t}_a = \frac{1}{N} \sum_{i=1}^N t_a(y_i)\).

We consider the Chebyshev inequalities for

\[
k = \frac{\sqrt{N} \lambda_{\min}(\mathcal{I}(\theta))}{\|\rho\|_2 \sqrt{\lambda_{\max}(\mathcal{I}(h_L))}} > 0.
\]

\[
\Pr \left( \| \bar{t} - E[\bar{t}] \|_2 \leq \frac{1}{N} \lambda_{\max}(\mathcal{I}(h_L)) \right)
= \Pr \left( \left\| \frac{\bar{t} - E[\bar{t}]}{\sqrt{\frac{1}{N} \lambda_{\max}(\mathcal{I}(h_L))}} \right\|_2 \leq k \right)
\geq \Pr \left( (\bar{t} - E[\bar{t}])^\top \left( \frac{1}{N} \mathcal{I}(h_L) \right)^{-1} (\bar{t} - E[\bar{t}]) \leq k^2 \right)
\geq 1 - \frac{n_L}{k^2}

= 1 - \frac{n_L \|\rho\|^2 \lambda_{\max}(\mathcal{I}(h_L))}{N \lambda_{\min}^2(\mathcal{I}(\theta))}.
\]

Thus with probability at least

\[
1 - \frac{n_L \|\rho\|^2 \lambda_{\max}(\mathcal{I}(h_L))}{N \lambda_{\min}^2(\mathcal{I}(\theta))},
\]

\[22\]
the following statement is true: for all unit vector $v$ we have

$$v^\top \hat{I}_2(\theta)v = v^\top \left( \mathcal{I}(\theta) - \sum_{a=1}^{n} (t_a - \mathbb{E}[t_a]) \frac{\partial^2 h^a_L(x)}{\partial \theta \partial \theta^\top} \right) v$$

$$= v^\top \mathcal{I}(\theta)v - \sum_{a=1}^{n} (t_a - \mathbb{E}[t_a]) \left( v^\top \frac{\partial^2 h^a_L(x)}{\partial \theta \partial \theta^\top} v \right)$$

$$\geq \lambda_{\text{min}}(\mathcal{I}(\theta)) - \sum_{a=1}^{n} (t_a - \mathbb{E}[t_a]) \left( v^\top \frac{\partial^2 h^a_L(x)}{\partial \theta \partial \theta^\top} v \right)$$

$$\geq \lambda_{\text{min}}(\mathcal{I}(\theta)) - \sum_{a=1}^{n} |t_a - \mathbb{E}[t_a]| \cdot \rho(\partial^2 h^a_L)$$

$$\geq \lambda_{\text{min}}(\mathcal{I}(\theta)) - k \cdot \sqrt{\frac{1}{n} \lambda_{\text{max}}(\mathcal{I}(h)_L)} \cdot \| \rho \|_2$$

$$\geq \lambda_{\text{min}}(\mathcal{I}(\theta)) - \lambda_{\text{min}}(\mathcal{I}(\theta))$$

$$= 0.$$ 

Thus with the specified probability, estimator $\hat{I}_2(\theta)$ is a positive semidefinite matrix. ☐

### B.11 Proof of Theorem 11

**Proof.** Let $t_a = \frac{1}{N} \sum_{i=1}^{N} t_a(y_i)$. As the FIM is a p.s.d. matrix, $\forall v$ such that $\|v\| = 1$, we have

$$v^\top \hat{I}_2(\theta)v = v^\top \left( \mathcal{I}(\theta) - \sum_{a=1}^{n} (t_a - \mathbb{E}[t_a]) \frac{\partial^2 h^a_L(x)}{\partial \theta \partial \theta^\top} \right) v$$

$$\geq -v^\top \left( (t_a - \mathbb{E}[t_a]) \frac{\partial^2 h^a_L(x)}{\partial \theta \partial \theta^\top} \right) v$$

$$= (\eta_a - \bar{t}_a) \cdot v^\top \left( \frac{\partial^2 h^a_L(x)}{\partial \theta \partial \theta^\top} \right) v$$

$$\geq -|\eta_a - \bar{t}_a| \cdot \rho(\partial^2 h^a_L) \cdot v^\top v$$

$$= -\rho(\partial^2 h^a_L) |\eta_a - \bar{t}_a|.$$ 

As $\hat{I}_2(\theta)$ is a real symmetric matrix, we can write its spectrum decomposition as

$$\hat{I}_2(\theta) = \hat{\lambda}^\alpha v_\alpha v_\alpha^\top,$$

where $\{v_\alpha\}$ are orthonormal vectors and $\hat{\lambda}^\alpha$ are the corresponding eigenvalues of $\hat{I}_2(\theta)$. Therefore

$$\hat{\lambda}^\alpha = v_\alpha^\top \hat{I}_2(\theta)v_\alpha \geq -\rho(\partial^2 h^a_L) |\eta_a - \bar{t}_a|.$$ 

The statement in Theorem 11 follows immediately. ☐

### B.12 Proof of Lemma 12

To prove the Lemma, we first consider a variant of the result presented in Chen [2007].
Lemma A.1 (Variant of Chen [2007]). For any random vector \( X \in \mathbb{R}^n \) with variances \( \text{Var}(X) \),

\[
\Pr \left( (X - E X)\top (X - E X) \geq \varepsilon \right) \leq \frac{1}{\varepsilon} \cdot \sum_{i=1}^{n} \text{Var}(X_i), \quad \forall \varepsilon > 0.
\]

**Proof.** The proofs follows closely to Chen [2007], with the slight change in set of variables considered. Let \( \varepsilon > 0 \) and \( D_\varepsilon := \{ V \in \mathbb{R}^n : (V - E X)\top (V - E X) \geq \varepsilon \} \). By definition we have that for all \( V \in D_\varepsilon \),

\[
(V - E X)\top (V - E X) \cdot \frac{1}{\varepsilon} \geq 1
\]

Thus for the probability of the set, we have:

\[
\Pr \left( (X - E X)\top (X - E X) \geq \varepsilon \right) = \Pr \left( X \in D_\varepsilon \right) \\
= \mathbb{E} \left[ 1_{X \in D_\varepsilon} \right] \\
\leq \frac{1}{\varepsilon} \cdot \mathbb{E} \left[ (X - E X)\top (X - E X) \cdot 1_{X \in D_\varepsilon} \right] \\
\leq \frac{1}{\varepsilon} \cdot \mathbb{E} \left[ (X - E X)\top (X - E X) \right] \\
= \frac{1}{\varepsilon} \cdot \sum_{i=1}^{n} \mathbb{E}[(X_i - E X_i)(X_i - E X_i)] \\
= \frac{1}{\varepsilon} \cdot \sum_{i=1}^{n} \text{Var}(X_i),
\]

where \( 1_{X \in S} \) denotes the indicator function for \( X \) being in a set \( S \). \( \square \)

We can now prove the main Lemma through standard tricks:

**Proof.** From Lemma A.1 (and utilizing the vec operator) we have that for any \( \delta > 0 \) and each \( z \in \{1, 2\} \):

\[
\Pr(\|\hat{I}_z(\theta) - I(\theta)\|_F^2 \leq \delta) \geq \frac{1}{\delta} \cdot \sum_{i,j=1}^{\text{dim}(\theta)} \text{Var} \left( \hat{I}_z(\theta) \right)^{ij}.
\]

Letting \( \varepsilon := \frac{1}{\delta} \cdot \sum_{i,j=1}^{\text{dim}(\theta)} \text{Var} \left( \hat{I}_z(\theta) \right)^{ij} \) and rearranging, we have:

\[
\Pr \left( \|\hat{I}_z(\theta) - I(\theta)\|_F \geq \frac{1}{\varepsilon} \cdot \sum_{i,j=1}^{\text{dim}(\theta)} \text{Var} \left( \hat{I}_z(\theta) \right)^{ij} \right) \leq 1 - \varepsilon
\]

\[
\Rightarrow \Pr \left( \|\hat{I}_z(\theta) - I(\theta)\|_F \geq \frac{1}{\sqrt{\varepsilon}} \cdot \sqrt{\sum_{i,j=1}^{\text{dim}(\theta)} \text{Var} \left( \hat{I}_z(\theta) \right)^{ij}} \right) \leq 1 - \varepsilon.
\]

Substituting appropriately from Eq. (10) w.r.t. the FIM estimator considered completes the proof. \( \square \)

**B.13 Proof of Lemma 13**

**Proof.** We first show that \( B_l \) is the Jacobian of the mapping \( h_l \rightarrow h_L \), that is,

\[
dh_L = B_l dh_l. \quad (l = 0, \cdots, L)
\]

(A.2)
Obviously, this is true for $l = L$, as we have

$$dh_L = I \cdot dh_L = B_L \cdot dh_L.$$  

From Eq. (3), we have

$$h_{l+1} = \sigma(W_l \bar{h}_l),$$

where $\sigma$ is abused to denote the non-linear activation function for $l = 0, \cdots, L - 2$ and $\sigma$ is the identity map for $l = L - 1$. Therefore

$$dh_{l+1} = D_l \cdot W_l^{-} \cdot dh_l,$$

where $D_l = \text{diag}(\sigma'(W_l \bar{h}_l))$ for $l = 0, \cdots, L - 2$, and $D_{L-1} = I$. Assume Eq. (A.2) is true for $l + 1$, then

$$dh_L = B_{l+1} dh_{l+1} = B_{l+1} \cdot D_l \cdot W_l^{-} \cdot dh_l = B_l dh_l.$$  

Hence $B_l$ is the Jacobian of $h_l \to h_L$ for $l = 0, \cdots, L$.

Now we are ready to derive the expression of $\frac{\partial \ell}{\partial h_l}$.

Next, we show the gradient w.r.t. the neural network weights, i.e. $\frac{\partial \ell}{\partial W_l}$. We have

$$d \ell = d(\log p(y | x))$$

$$= d\{t^\top (y) h_L - F(h_L)\}$$

$$= \text{tr}\{d\{t^\top (y) h_L - F(h_L)\}\}$$

$$= \text{tr}\{d\{t^\top (y) h_L - F(h_L)\}\}$$

$$= \text{tr}\{d\{t^\top (y) d h_L - \nabla F(h_L)^\top d h_L\}\}$$

$$= \text{tr}\{t^\top (y) dh_L - \eta^\top (h_L) dh_L\}$$

$$= \text{tr}\{(t(y) - \eta(h_L))^\top B_l dh_l\}$$

Therefore

$$\frac{\partial \ell}{\partial h_l} = (t(y) - \eta(h_L))^\top B_l = B_l^\top (t(y) - \eta(h_L)).$$

Next, we show the gradient w.r.t. the neural network weights, i.e. $\frac{\partial \ell}{\partial W_l}$. We have

$$d \ell = \text{tr}\left\{\left(\frac{\partial \ell}{\partial h_{l+1}}\right)^\top dh_{l+1}\right\}$$

$$= \text{tr}\left\{\left(\frac{\partial \ell}{\partial h_{l+1}}\right)^\top D_l \cdot dW_l \cdot \bar{h}_l\right\}$$

$$= \text{tr}\left\{h_l \left(\frac{\partial \ell}{\partial h_{l+1}}\right)^\top D_l \cdot dW_l\right\}.$$
Therefore
\[
\frac{\partial \ell}{\partial W_l} = \left( \bar{h}_l \left( \frac{\partial \ell}{\partial h_{l+1}} \right)^\top D_l \right)^\top \\
= D_l^\top \left( \frac{\partial \ell}{\partial h_{l+1}} \right) \bar{h}_{l+1}^\top \\
= D_l \left( \frac{\partial \ell}{\partial h_{l+1}} \right) \bar{h}_{l+1}^\top.
\]

Finally, we give the gradient of \( h_L \) w.r.t. the neural network parameters. By definition, \( B_{l+1} \) is the Jacobian of the mapping \( h_{l+1} \rightarrow h_L \). Therefore
\[
dh_L = B_{l+1} \cdot dh_{l+1} = B_{l+1} \cdot D_l \cdot dW_l \cdot \bar{h}_l.
\]

We rewrite the above equation in the element-wise form
\[
dh_L^a = \text{tr} \left\{ B_{l+1} \cdot D_l \cdot dW_l \cdot \bar{h}_l e_a^\top \right\} \\
= \text{tr} \left\{ h_l e_a^\top B_{l+1} \cdot D_l \cdot dW_l \right\}.
\]

Therefore
\[
\frac{\partial h_L^a}{\partial W_l} = \left( h_l e_a^\top B_{l+1} \cdot D_l \right)^\top \\
= D_l^\top B_{l+1} e_a \bar{h}_l^\top \\
= D_l B_{l+1} e_a \bar{h}_l^\top.
\]

\[ \Box \]

**B.14 Proof of Lemma 14**

**Proof.** First, we notice that
\[
\frac{\partial h_L^a}{\partial W_l} = D_l B_{l+1}^\top e_a \cdot \bar{h}_l^\top
\]
has rank one. Therefore
\[
\left\| \frac{\partial h_L^a}{\partial W_l} \right\|_F = \left\| D_l B_{l+1}^\top e_a \right\|_2 \cdot \left\| \bar{h}_l \right\|_2.
\]

Therefore
\[
\left\| \frac{\partial h_L}{\partial W_l} \right\|_F = \sqrt{\sum_a \left\| \frac{\partial h_L^a}{\partial W_l} \right\|_F^2} = \sqrt{\sum_a \left\| D_l B_{l+1}^\top e_a \right\|_2 \cdot \left\| \bar{h}_l \right\|_2^2} \\
= \sqrt{\sum_a \left\| D_l B_{l+1}^\top e_a \right\|_2 \cdot \left\| \bar{h}_l \right\|_2} \\
= \left\| D_l B_{l+1} \right\|_F \cdot \left\| \bar{h}_l \right\|_2 \\
= \left\| B_{l+1} \cdot D_l \right\|_F \cdot \left\| \bar{h}_l \right\|_2.\]
The matrix $D_l$ is diagonal, with entries bounded in the range $[-1, 1]$. Therefore a left or right multiplication by $D_l$ does not increase the Frobenius norm. Hence

$$\left\| \frac{\partial h_L}{\partial W_l} \right\|_F \leq \| B_{l+1} \|_F \cdot \| \delta h_l \|_2.$$ 

By the recursive definition of $B_l$, we have

$$B_l = B_{l+1} D_l W_l^-. $$

Therefore

$$\| B_l \|_F \leq \| B_{l+1} \|_F \cdot \| D_l W_l^- \|_F \leq \| B_{l+1} \|_F \cdot \| W_l^- \|_F.$$ 

Applying the above inequality repeatably leads to

$$\| B_l \|_F \leq \| B_{L-1} \|_F \cdot \prod_{i=l}^{L-2} \| W_i^- \|_F$$

$$= \| B_L D_{L-1} W_{L-1}^- \|_F \cdot \prod_{i=l}^{L-2} \| W_i^- \|_F$$

$$= \| W_{L-1}^- \|_F \cdot \prod_{i=l}^{L-2} \| W_i^- \|_F$$

$$= \prod_{i=l}^{L-1} \| W_i^- \|_F.$$ 

Hence

$$\left\| \frac{\partial h_L}{\partial W_l} \right\|_F \leq \| B_{l+1} \|_F \cdot \| \delta h_l \|_2$$

$$\leq \prod_{i=l+1}^{L-1} \| W_i^- \|_F \cdot \| \delta h_l \|_2.$$ 

\[ \square \]

**B.15 Proof of Lemma 15**

**Proof.** Recall the 2-spectral norm for a $d$-dimensional tensor is defined by

$$\| T \|_{2^*} = \max \left\{ \langle T, x^1 \otimes \ldots \otimes x^d \rangle : \| x^k \|_2 = 1, \forall k \in [d] \right\}.$$ 

Let $\alpha, \beta, \gamma$ be unit vectors, so that

$$\| \alpha \|_2 = 1, \quad \| \beta \|_2 = 1, \quad \| \gamma \|_2 = 1.$$ 

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Then
\[
\max_{\alpha, \beta, \gamma} \left\langle \frac{\partial h}{\partial W}, \alpha \otimes \beta \otimes \gamma \right\rangle = \max_{\alpha, \beta, \gamma} \left\langle \sum_a \frac{\partial h_a}{\partial W} g_a, \alpha \otimes \beta \right\rangle
\]
\[
= \max_{\alpha, \beta, \gamma} \sum_a \alpha^T D_i B_i^T \gamma_a h_i^T \beta \gamma_a
\]
\[
= \max_{\alpha, \beta, \gamma} \alpha^T D_i B_i^T \gamma (h_i^T \beta)
\]
\[
= \max_{\alpha, \beta, \gamma} \langle B_{i+1} D_i \alpha, \gamma \rangle \cdot \langle h_i, \beta \rangle
\]
\[
= \max_{\alpha} \| B_{i+1} D_i \alpha \|_2 \cdot \| h_i \|_2.
\]

Recall that
\[
B_l = B_{i+1} D_i W_i^{-}.
\]

Therefore
\[
B_l D_{l-1} \alpha = B_{i+1} D_i W_i^{-} D_{l-1} \alpha.
\]

Moreover,
\[
\max_{\alpha} \| B_l D_{l-1} \alpha \|_2 = \max_{\alpha} \max_{\alpha'} \| B_{i+1} D_i W_i^{-} D_{l-1} \alpha' \|_2
\]
\[
\leq \max_{\alpha'} \max(s_{\text{max}}(W_i^{-})), \| B_{i+1} D_i \alpha' \|_2
\]
\[
= \max(s_{\text{max}}(W_i^{-})) \max_{\alpha'} \| B_{i+1} D_i \alpha' \|_2.
\]

Hence,
\[
\max_{\alpha, \beta, \gamma} \left\langle \frac{\partial h}{\partial W}, \alpha \otimes \beta \otimes \gamma \right\rangle = \max_{\alpha} \| B_{i+1} D_i \alpha \|_2 \cdot \| h_i \|_2
\]
\[
\leq \prod_{i=L}^{L-1} s_{\text{max}}(W_i^{-}) \max_{\alpha'} \| B_L D_{L-1} \alpha' \|_2 \cdot \| h_i \|_2
\]
\[
= \prod_{i=L+1}^{L-1} s_{\text{max}}(W_i^{-}) \max_{\alpha} \| B_L D_{L-1} \alpha \|_2 \cdot \| h_i \|_2
\]
\[
= \prod_{i=L+1}^{L-1} s_{\text{max}}(W_i^{-}) \max_{\alpha} \| I \alpha \|_2 \cdot \| h_i \|_2
\]
\[
= \prod_{i=L+1}^{L-1} s_{\text{max}}(W_i^{-}) \max_{\alpha} \| \alpha \|_2 \cdot \| h_i \|_2
\]
\[
= \prod_{i=L+1}^{L-1} s_{\text{max}}(W_i^{-}) \cdot \| h_i \|_2.
\]
C Change of Coordinates and Covariance

Reparametrization is a common technique in deep learning. See e.g. weight normalization [Salimans and Kingma, 2016]. From a geometric perspective, reparametrization corresponds to change of coordinates. We consider how our results can be generalized in a new coordinate system \( \{ \xi_i \} \) instead of the default coordinates \( \{ \theta_i \} \). By definition, the FIM w.r.t. to the new coordinates is

\[
\mathcal{I}(\xi) = \frac{\partial \theta_\alpha}{\partial \xi^a} \frac{\partial h_L^\alpha}{\partial \theta^\alpha} \mathcal{I}_{\alpha\beta}(h_L) \frac{\partial h_L^\beta}{\partial \theta^\beta} \frac{\partial \theta_\beta}{\partial \xi^b} = \frac{\partial \theta_\alpha}{\partial \xi^a} \mathcal{I}^{ab}(\theta) \frac{\partial \theta_\beta}{\partial \xi^b}.
\]

(A.3)

The FIM \( \mathcal{I}(\xi) \) can be estimated by Eq. (2), where the estimators are denoted by \( \hat{\mathcal{I}}_1(\xi) \) and \( \hat{\mathcal{I}}_2(\xi) \).

Note that as per the main text, upper- and lower-indices in the Einstein are equivalent. Similarly, we take an upper index for derivatives of \( h_L \) w.r.t. \( \theta \) in this section — which we take as equivalent to the lower-index notation appearing in the main text. That is \( \partial^2 h_L = \partial h_L / \partial \theta^\alpha = \partial h_L / \partial \theta^\beta \).

**Theorem A.2.** Consider the FIM estimators under the coordinate transformation \( \theta \rightarrow \xi \) with the same samples size \( N \).

\[
\hat{\mathcal{I}}_1(\xi) = \frac{\partial \theta_\alpha}{\partial \xi^a} \hat{\mathcal{I}}_1^{ab}(\theta) \frac{\partial \theta_\beta}{\partial \xi^b},
\]

(A.4)

\[
\hat{\mathcal{I}}_2(\xi) = \frac{\partial \theta_\alpha}{\partial \xi^a} \hat{\mathcal{I}}_2^{ab}(\theta) \frac{\partial \theta_\beta}{\partial \xi^b} + \left( \eta_\alpha - \frac{1}{N} \sum_{i=1}^{N} t_\alpha(y_i) \right) \frac{\partial^2 h_L^\alpha}{\partial \xi^a \partial \xi^b} \frac{\partial^2 \theta_\beta}{\partial \xi^b}.
\]

(A.5)

**Proof.** Let \( \hat{E}[X] \) denote the empirical expectation of random variable \( X \).

For the first estimator, consider the partial derivative of the log-likelihood:

\[
\frac{\partial \ell}{\partial \xi} = \left( \frac{\partial \ell}{\partial \xi} \right)^\top \left( \frac{\partial \ell}{\partial \theta} \right) = \frac{\partial \theta_\alpha}{\partial \xi^a} \frac{\partial h_L^\alpha}{\partial \theta^\alpha} \frac{\partial h_L^\beta}{\partial \theta^\beta} \frac{\partial \theta_\beta}{\partial \xi^b} (t_\alpha(y) - \eta_\alpha).
\]

Thus the first FIM estimator follows immediately:

\[
\hat{E} \left[ \frac{\partial \ell}{\partial \xi} \frac{\partial \ell}{\partial \xi^\top} \right] = \hat{E} \left[ \frac{\partial \theta_\alpha}{\partial \xi^a} \frac{\partial h_L^\alpha}{\partial \theta^\alpha} (t_\alpha(y) - \eta_\alpha) \frac{\partial h_L^\beta}{\partial \theta^\beta} (t_\beta(y) - \eta_\beta) \right] = \frac{\partial \theta_\alpha}{\partial \xi^a} \hat{E} \left[ \frac{\partial h_L^\alpha}{\partial \theta^\alpha} (t_\alpha(y) - \eta_\alpha) \frac{\partial h_L^\beta}{\partial \theta^\beta} (t_\beta(y) - \eta_\beta) \right] \frac{\partial \theta_\beta}{\partial \xi^b} = \frac{\partial \theta_\alpha}{\partial \xi^a} \hat{\mathcal{I}}_1(\theta) \frac{\partial \theta_\beta}{\partial \xi^b}.
\]

For the second estimator, we consider the second derivative:

\[
\frac{\partial^2 \ell}{\partial \xi \partial \xi^\top} = \frac{\partial}{\partial \xi} \left[ \frac{\partial \theta_\alpha}{\partial \xi^a} \frac{\partial h_L^\alpha}{\partial \theta^\alpha} (t_\alpha(y) - \eta_\alpha) \right] = -\frac{\partial \eta_\alpha}{\partial \xi} \frac{\partial h_L^\alpha}{\partial \theta^\alpha} \frac{\partial \theta_\alpha}{\partial \xi^a} + (t_\alpha - \eta_\alpha) \left[ \frac{\partial}{\partial \xi} \left( \frac{\partial h_L^\alpha}{\partial \theta^\alpha} \right) \frac{\partial \theta_\alpha}{\partial \xi^a} + (t_\alpha - \eta_\alpha) \frac{\partial^2 h_L^\alpha}{\partial \theta^\alpha \partial \theta^\alpha} \frac{\partial \theta_\alpha}{\partial \xi^a} \right]
\]

\[
= -\frac{\partial \theta_\beta}{\partial \xi} \left[ \frac{\partial h_L^\alpha}{\partial \theta^\alpha} \frac{\partial \eta_\alpha}{\partial \theta^\alpha} \frac{\partial h_L^\alpha}{\partial \theta^\alpha} (t_\alpha - \eta_\alpha) \right] \frac{\partial \theta_\beta}{\partial \xi^b} = \frac{\partial \theta_\beta}{\partial \xi^b} \frac{\partial^2 \theta_\beta}{\partial \theta^\alpha \partial \theta^\alpha} \frac{\partial \theta_\alpha}{\partial \xi^a} + (t_\alpha - \eta_\alpha) \frac{\partial^2 \theta_\beta}{\partial \theta^\alpha \partial \theta^\alpha} \frac{\partial \theta_\alpha}{\partial \xi^a}.
\]
Theorem A.3. Thus we have both estimators for the theorem. Taking the empirical expectation we have:

\[
\hat{E} \left[ -\frac{\partial^2 \ell}{\partial \xi \partial \xi^\top} \right] = \hat{E} \left[ \frac{\partial \theta_a}{\partial \xi} \left[ \frac{\partial [h_L]_b}{\partial \theta^a} \frac{\partial \eta_a}{\partial \theta^b} \frac{\partial h_b^\top}{\partial \theta^a} \right] \right] \frac{\partial \theta_a}{\partial \xi} = \hat{E} \left[ \frac{\partial [h_L]_b}{\partial \theta^a} \frac{\partial \eta_a}{\partial \theta^b} \frac{\partial h_b^\top}{\partial \theta^a} \right] + \hat{E} \left[ \frac{\partial [h_L]_b}{\partial \theta^a} \frac{\partial \eta_a}{\partial \theta^b} \frac{\partial h_b^\top}{\partial \theta^a} \right] - \hat{E} \left[ \frac{\partial [h_L]_b}{\partial \theta^a} \frac{\partial \eta_a}{\partial \theta^b} \frac{\partial h_b^\top}{\partial \theta^a} \right] \frac{\partial \theta_a}{\partial \xi} \frac{\partial \theta_a}{\partial \xi^\top} + \hat{E} \left[ \frac{\partial [h_L]_b}{\partial \theta^a} \frac{\partial \eta_a}{\partial \theta^b} \frac{\partial h_b^\top}{\partial \theta^a} \right] \frac{\partial \theta_a}{\partial \xi} \frac{\partial \theta_a}{\partial \xi^\top}.
\]

Thus we have both estimators for the theorem.

Interestingly, the way to compute \( \hat{I}_1(\xi) \) under coordinate transformation follows the same rule to compute the FIM \( \hat{I}(\xi) \) in the new coordinate system. See the similarity between Eq. (A.3) and Eq. (A.4). The transformation rule of \( \hat{I}_2(\xi) \) introduces an additional term, which depends on the Hessian of the coordinate transform \( \partial^2 \theta_\beta/\partial \xi \partial \xi^\top \). This term vanishes as the number of samples increases \( N \to \infty \), or the transformation \( \theta \to \xi \) is affine.

The results we need to generalize for coordinate transformation depend on the (co)variance of the estimators. As such, we present a \( \{\xi_i\} \) variant of Theorems 4 and 6.

**Theorem A.3.**

\[
\begin{bmatrix}
\text{Cov} (\hat{I}_1(\xi)) \\
\text{Cov} (\hat{I}_2(\xi))
\end{bmatrix}_{ijkl} = \begin{bmatrix}
\frac{\partial \theta_a}{\partial \xi_i} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial \theta_c}{\partial \xi_k} \frac{\partial \theta_d}{\partial \xi_l} \text{Cov} (\hat{I}_1(\theta))_{abcd} \\
\frac{\partial \theta_a}{\partial \xi_i} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial \theta_c}{\partial \xi_k} \frac{\partial \theta_d}{\partial \xi_l} \text{Cov} (\hat{I}_2(\theta))_{abcd} + \frac{1}{N} C^{\alpha \beta} \text{I}_{\alpha \beta}(h_L)
\end{bmatrix}
\]

where \( C^{\alpha \beta} := \)

\[
\frac{\partial^3 \theta_a}{\partial \xi_i \partial \xi_j \partial \xi_k} \partial^\alpha h_L^\top \partial^\beta h_L^\top + \frac{\partial^3 \theta_a}{\partial \xi_i \partial \xi_j \partial \xi_k} \partial^\alpha h_L^\top \partial^\beta h_L^\top + \frac{\partial^3 \theta_a}{\partial \xi_i \partial \xi_j \partial \xi_k} \partial^\alpha h_L^\top \partial^\beta h_L^\top.
\]

**Proof.** For the first estimator’s covariance, immediately get the result by the way covariance interacts with constant products:

\[
\text{Cov} \left( [\hat{I}_1(\xi)]^{ij}, [\hat{I}_1(\xi)]^{kl} \right) = \text{Cov} \left( \frac{\partial \theta_a}{\partial \xi_i} [\hat{I}_1(\theta)]^{ab}, \frac{\partial \theta_b}{\partial \xi_j} [\hat{I}_1(\theta)]^{cd}, \frac{\partial \theta_c}{\partial \xi_k} [\hat{I}_1(\theta)]^{ad}, \frac{\partial \theta_d}{\partial \xi_l} [\hat{I}_1(\theta)]^{bd} \right)
\]

\[
= \frac{\partial \theta_a}{\partial \xi_i} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial \theta_c}{\partial \xi_k} \frac{\partial \theta_d}{\partial \xi_l} \text{Cov} \left( [\hat{I}_1(\theta)]^{ab}, [\hat{I}_1(\theta)]^{cd} \right)
\]

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For the second estimator, we must exploit the linear combination property of covariances as well:

\[
\text{Cov}\left(\hat{\mathcal{I}}_2(\xi)^{ij}, [\hat{\mathcal{I}}_2(\xi)]^{kl}\right)
\]

\[
= \text{Cov}\left(\frac{\partial \theta_a}{\partial \xi_i} [\hat{\mathcal{I}}_2(\theta)]^{ab} \frac{\partial \theta_b}{\partial \xi_j} + \left(\eta_a - \frac{1}{N} \sum_{i=1}^{N} t_a(y_i)\right) \frac{\partial^2 \theta_a}{\partial \theta^a \partial \xi_i} \frac{\partial^2 \theta_b}{\partial \theta^b \partial \xi_j}, \right)
\]

\[
\frac{\partial \theta_c}{\partial \xi_k} \frac{\partial \theta_d}{\partial \xi_l} + \left(\eta_b - \frac{1}{N} \sum_{i=1}^{N} t_b(y_i)\right) \frac{\partial h_L^a}{\partial \theta^a} \frac{\partial h_L^b}{\partial \theta^b} \right)
\]

\[
+ \text{Cov}\left(\eta_a - \frac{1}{N} \sum_{i=1}^{N} t_a(y_i), \frac{\partial h_L^a}{\partial \theta^a} \frac{\partial^2 \theta_d}{\partial \theta^d \partial \xi_k \partial \xi_l}\right)
\]

\[
+ \text{Cov}\left(\eta_b - \frac{1}{N} \sum_{i=1}^{N} t_b(y_i), \frac{\partial h_L^b}{\partial \theta^b} \frac{\partial^2 \theta_d}{\partial \theta^d \partial \xi_k \partial \xi_l}\right)
\]

It follows that the first covariance term is exactly the coordinate transform of the original variance:

\[
\text{Cov}\left(\frac{\partial \theta_a}{\partial \xi_i} [\hat{\mathcal{I}}_2(\theta)]^{ab} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial \theta_c}{\partial \xi_k} [\hat{\mathcal{I}}_2(\theta)]^{cd} \frac{\partial \theta_d}{\partial \xi_l}\right) = \frac{\partial \theta_a}{\partial \xi_i} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial \theta_c}{\partial \xi_k} \frac{\partial \theta_d}{\partial \xi_l} \text{Cov}\left(\hat{\mathcal{I}}_2(\theta)^{ab}, \hat{\mathcal{I}}_2(\theta)^{cd}\right).
\]

For the final covariance term we have:

\[
\text{Cov}\left(\eta_a - \frac{1}{N} \sum_{i=1}^{N} t_a(y_i), \frac{\partial h_L^a}{\partial \theta^a} \frac{\partial \theta_d}{\partial \xi_k \partial \xi_l}\right)
\]

\[
= \frac{\partial^2 \theta_a}{\partial \xi_i \partial \xi_j \partial \theta^a} \text{Cov}\left(\frac{\partial h_L^a}{\partial \theta^a} \frac{\partial \theta_d}{\partial \xi_k \partial \xi_l}\right)
\]

\[
= \frac{\partial^2 \theta_a}{\partial \xi_i \partial \xi_j \partial \theta^a} \frac{\partial h_L^a}{\partial \theta^a} \frac{\partial h_L^a}{\partial \theta^a} \text{Cov}\left(\frac{\partial \theta_d}{\partial \xi_k \partial \xi_l}\right)
\]

\[
= \frac{\partial^2 \theta_a}{\partial \xi_i \partial \xi_j \partial \theta^a} \frac{\partial h_L^a}{\partial \theta^a} \frac{\partial h_L^a}{\partial \theta^a} \frac{1}{N} \sum_{i=1}^{N} \text{Cov}\left(\eta_a - t_a(y_i), \eta_b - t_b(y_i)\right)
\]

where the second last line comes from the independence of samples.
Thus all there is left is to calculate the middle terms. Without loss of generality, we calculate:

\[
\text{Cov} \left( \frac{\partial \theta_a}{\partial \xi_i}, [\hat{\xi}_2(\theta)]_{ab}, \text{Cov} \left( \eta, \frac{1}{N} \sum_{i=1}^{N} t_\beta(y_i) \frac{\partial h_L^2}{\partial \theta^\beta}, \frac{\partial^2 \theta_b}{\partial \xi_j \partial \xi_k} \right) \right)
\]

\[
= \frac{\partial \theta_a}{\partial \xi_i} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial^2 \theta_c}{\partial \xi_k \partial \xi_l} \text{Cov} \left( [\hat{\xi}_2(\theta)]_{ab}, \left( \frac{1}{N} \sum_{i=1}^{N} t_\beta(y_i) \right) \frac{\partial h_L^2}{\partial \theta^\beta} \right)
\]

\[
= \frac{\partial \theta_a}{\partial \xi_i} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial^2 \theta_c}{\partial \xi_k \partial \xi_l} \text{Cov} \left( \frac{1}{N} \sum_{i=1}^{N} t_\beta(y_i), \left( \frac{1}{N} \sum_{i=1}^{N} t_\beta(y_i) \right) \frac{\partial h_L^2}{\partial \theta^\beta} \right)
\]

\[
= \frac{\partial \theta_a}{\partial \xi_i} \frac{\partial \theta_b}{\partial \xi_j} \frac{\partial^2 \theta_c}{\partial \xi_k \partial \xi_l} \frac{1}{N} \text{I}_{\eta,\beta}(h_L).
\]

Combining these 3 covariance results gives us the covariance presented in the theorem. \(\square\)

As per the estimators themselves in Theorem A.2, the 4D covariances obey similar rules under coordinate transformations. Equation (A.7) has an additional term \(\frac{1}{N} \text{Cov} \cdot \text{I}_{\eta,\beta}(h_L)\) which depends on the Hessian of the coordinate transformation. Notice that each of the coordinate transformed covariance values depend on the same central moments of the exponential family – even the second estimator with the additional term only depends on the covariance/FIM w.r.t. \(h_L\). Each of these covariances include a weighted sums of the original covariance matrices in Theorems 4 and 6. As such, our initial element-wise considerations of the covariance will still be useful in the computation of the covariance in the new coordinates. In-fact, our upper bounds in Lemmas A.4 and A.5 and Theorem A.6 can be simply adapted by adding the appropriate norms of the coordinate transformation (and its Hessian component for the second estimator).

## D Element-wise Covariance Bounds

The covariance tensor \(\text{Cov} \left( \hat{\xi}_1(\theta) \right) \) has the following element-wise bound.

**Lemma A.4.**

\[
\left| \text{Cov} \left( \hat{\xi}_1(\theta) \right) \right|_{ijkl} \leq \frac{1}{N} \sum_{i=1}^{N} \parallel \partial_i h_L(x) \parallel_2 \cdot \parallel \partial_j h_L(x) \parallel_2 \cdot \parallel \partial_k h_L(x) \parallel_2 \cdot \parallel \partial_l h_L(x) \parallel_2 \cdot \parallel \text{K}(t) - \text{T}(h_L) \otimes \text{T}(h_L) \parallel_F,
\]

where \(\parallel \cdot \parallel_F\) is the Frobenius norm of a tensor (square root of the sum of the squares of the elements / the L2-norm) and \(\otimes\) is the tensor-product: \((\text{T}(h_L) \otimes \text{T}(h_L))_{abcd} := \text{T}(h_L) \cdot \text{T}(h_L)\).

**Proof.** Corollary holds immediately from the use of Hölder’s inequality / Cauchy-Schwarz. Let \(1 \leq p, q \leq 32\).
∞ such that 1/p + 1/q = 1. Let \( T_{abcd} = K_{abcd}(t) - \mathcal{I}_{ab}(h_L) \cdot \mathcal{I}_{cd}(h_L) \). From Theorem 4 we have:

\[
\left| \text{Cov} \left( \hat{I}_1(\theta) \right) \right|_{ijkl} = \frac{1}{N} \cdot \left| \partial_i h_L^k(x) \partial_j h_L^l(x) \partial_k h_L^a(x) \partial_l h_L^b(x) \cdot T_{abcd} \right|
\]

\[
= \frac{1}{N} \cdot \| \partial_i h_L(x) \otimes \partial_j h_L(x) \otimes \partial_k h_L(x) \otimes \partial_l h_L(x) \|_p \cdot \| T \|_q
\]

\[
= \frac{1}{N} \cdot \| \partial_i h_L(x) \|_p \cdot \| \partial_j h_L(x) \|_p \cdot \| \partial_k h_L(x) \|_p \cdot \| \partial_l h_L(x) \|_p \cdot \| T \|_q.
\]

Thus, by taking the \( p = q = 2 \) the Lemma holds.

We have similar element-wise and global upper bounds on the covariance of \( \hat{I}_2(\theta) \).

**Lemma A.5.**

\[
\left| \text{Cov} \left( \hat{I}_2(\theta) \right) \right|_{ijkl} \leq \frac{1}{N} \cdot \| \partial_i h_L^a(x) \partial_j h_L^b(x) \partial_k h_L^c(x) \partial_l h_L^d(x) \|_2 \cdot \| I(h_L) \|_F.
\]

**Proof.** Corollary holds immediately from the use of Hölder’s inequality / Cauchy-Schwarz. Let \( 1 \leq p, q \leq \infty \) such that \( 1/p + 1/q = 1 \). From Theorem 6 we have:

\[
\left| \text{Cov} \left( \hat{I}_2(\theta) \right) \right|_{ijkl} = \frac{1}{N} \cdot \left| \partial_i h_L^a(x) \partial_j h_L^b(x) \partial_k h_L^c(x) \partial_l h_L^d(x) \right|
\]

\[
= \frac{1}{N} \cdot \| \partial_i h_L(x) \otimes \partial_j h_L(x) \otimes \partial_k h_L(x) \|_p \cdot \| I(h_L) \|_q
\]

\[
= \frac{1}{N} \cdot \| \partial_i h_L(x) \|_p \cdot \| \partial_j h_L(x) \|_p \cdot \| \partial_k h_L(x) \|_p \cdot \| \partial_l h_L(x) \|_p \cdot \| I(h_L) \|_q.
\]

Thus, by taking the \( p = q = 2 \) the Lemma holds.

--

**E Alternative Norm Results**

An alternative bound to Theorem 7 and Theorem 8 can be established by utilizing Hölder’s inequality for \( L_p \)-norms.

**Theorem A.6.**

\[
\| \text{Cov} \left( \hat{I}_1(\theta) \right) \|_\infty \leq \frac{1}{N} \cdot \| h_L(x) \|_4^4 \cdot \| K(t) - I(h_L) \otimes I(h_L) \|_1 \quad (A.8)
\]

\[
\| \text{Cov} \left( \hat{I}_2(\theta) \right) \|_\infty \leq \frac{1}{N} \cdot \| h_L(x) \|_4^2 \cdot \| I(h_L) \|_1, \quad (A.9)
\]

where \( \| \cdot \|_\infty \) is the \( L_\infty \)-norm and \( \| \cdot \|_1 \) is the \( L_1 \)-norm.

**Proof.** The Corollary holds directly from the inequalities given in the proof of Theorem 7 and Theorem 8. Let \( p = \infty \) and \( q = 1 \).

Thus we have the inequalities for \( L_p \)-norms:

\[
\| \text{Cov} \left( \hat{I}_1(\theta) \right) \|_\infty \leq \frac{1}{N} \cdot \| h_L(x) \|_4^4 \cdot \| K(t) - I(h_L) \otimes I(h_L) \|_1
\]

\[
\| \text{Cov} \left( \hat{I}_2(\theta) \right) \|_\infty \leq \frac{1}{N} \cdot \| h_L(x) \|_4^2 \cdot \| I(h_L) \|_1.
\]

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Remark A.6.1. Note that these are exactly equivalent to certain spectral and nuclear norms. However these have slight differences in their definition [Chen and Li, 2020].

The standard tensor nuclear norm is only equivalent when \( p \) is even. The standard tensor spectral norm is only equivalent when \( p = 2 \).

We consider a convex combination of estimators, i.e., Eqs. (7) and (8).

Thus the analysis in Lemma 9 can be useful to extend the bounds in Theorem A.6. On the other hand, for the \( \| \cdot \|_{\alpha} \) and \( \| \cdot \|_{\lambda} \) we can upper bound it by the corresponding \( L_2 \)-norm through Cauchy-Schwarz, i.e., \( \| \cdot \|_1 \leq \| \cdot \|_2 \sqrt{D} \), where \( D(\cdot) \) is the product of the dimension size of the tensor. One should note that \( L_2 \) is the Frobenius norm.

\[
\| T \|_{\alpha} = \min \left\{ \sum_{i=1}^{r} |\lambda_i| : T = \sum_{i=1}^{r} \lambda_i x_i^1 \otimes \ldots \otimes x_i^d : \| x_i^k \|_p = 1, \forall k \in [d] \text{ and } i, r \in \mathbb{N} \right\}.
\]

Notably, the \( L_1 \)-norm can be upper-bounded by the Frobenius norm trivially through the Cauchy-Schwarz inequality, with \( \| \cdot \|_1 \leq \| \cdot \|_F \sqrt{D} \), where \( D \) is the product of the dimension size of the tensor. Thus the analysis in Lemma 9 can be useful to extend the bounds in Theorem A.6. On the other hand, the \( L_\infty \)-norm \( \| \cdot \|_\infty \) is upper bounded by the largest singular value of the tensor [Lim, 2005]. As such, the \( \| \cdot \|_\infty \) quantities on the RHS can be interpreted as functions of the maximum singular value of the Jacobian \( \partial h_L(x) \) or the Hessian \( \partial^2 h_L(x) \). Similar corollaries for Lemma A.4 and Lemma A.5 can be established — which we omit for brevity.

F Combination of Estimators

We consider a convex combination of estimators, i.e., Eqs. (7) and (8).

In particular, for \( 0 \leq \alpha \leq 1 \) we have:

\[
\hat{L}_\alpha(\theta) = \alpha \hat{L}_1(\theta) + (1 - \alpha) \hat{L}_2(\theta).
\]

(A.10)

Clearly, this is also a point-wise estimator. Thus, Proposition 1 holds for this estimator.

For the variance, we use the following linear relation:

\[
\text{Var}(\alpha \hat{L}_1(\theta) + (1 - \alpha) \hat{L}_2(\theta)) = \alpha^2 \text{Var}(\hat{L}_1(\theta)) + (1 - \alpha)^2 \text{Var}(\hat{L}_2(\theta)) + 2\alpha(1 - \alpha)\text{Cov}(\hat{L}_1(\theta), \hat{L}_2(\theta)).
\]

Or as we have previously discussed we consider:

\[
\alpha^2 \text{Var} \left( \frac{\partial \ell}{\partial \theta_i}, \frac{\partial \ell}{\partial \theta_j} \right) + (1 - \alpha)^2 \text{Var} \left( -\frac{\partial^2 \ell}{\partial \theta_i \partial \theta_j} \right) + 2\alpha(1 - \alpha)\text{Cov} \left( \frac{\partial \ell}{\partial \theta_i}, \frac{\partial \ell}{\partial \theta_j}, -\frac{\partial^2 \ell}{\partial \theta_i \partial \theta_j} \right)
\]

We already have the variance values from Theorems 4 and 6. Thus all we have to calculate is the covariance term.
We consider the MNIST dataset of 28 × 28 pixel grayscale images after normalization. The training set consists of 60,000 examples and the test set consists of 10,000 examples.

The covariance of the combined estimator:

\[ \alpha^2 \partial_a h^a_L \partial_i h^i_L \partial_j h^j_L \partial_k h^k_L \cdot (K_{abcd}(t) - I_{abcd}(h_L) \cdot I_{cd}(h_L)) + (1 - \alpha)^2 \partial_a h^a_L \partial_b h^b_L \partial_c h^c_L \cdot I_{a\beta}(h_L) \]

\[ - 2\alpha (1 - \alpha) \partial_a h^a_L \partial_b h^b_L \partial_c h^c_L \cdot E [\delta_a \cdot \delta_b \cdot \delta_c]. \]  

(A.11)

The covariance (as per Theorems 4 and 6) can similarly be calculated by changing the variables of the partial derivatives of \( h_L \). Notably, the largest differentiating factor from the original estimator is that the combined estimator is dependent on the third central moment of \( t \). This third central moment is equivalent to the third-order cumulant of \( t \). Thus it can be directly calculated via the derivatives of the log-partition function \( F(h_L) \).

**G  Experimental Verification of Bounds**

The bounds of the variance of the FIM estimators \( \hat{I}_1(\theta) \) and \( \hat{I}_2(\theta) \) (as presented in Section 3) can be experimentally verified. We train a simple convolutional neural network trained on the standard MNIST dataset. By leveraging the Jacobian and Hessian in-built functions in PyTorch, we calculate the bounds in Theorems 7 and 8 applied to the variance of the estimators (as described in Section 3.1).

**G.1 Dataset**

We consider the MNIST dataset of 28 × 28 pixel grayscale images after normalization. The training set consists of 60,000 examples and the test set consists of 10,000 examples.
G.2 Model Setup

The convolutional neural network considered in our experiments are given by the following layers (in order):

→ Conv(in_channel=1, out_channel=32, kernel_size=(3, 3), stride=(1, 1))
→ Softplus()
→ Conv(in_channel=32, out_channel=64, kernel_size=(3, 3), stride=(1, 1))
→ Softplus()
→ MaxPool2D()
→ Dropout(p=0.25)
→ Linear(in_features=9216, out_features=128)
→ Softplus()
→ Dropout(p=0.5)
→ Linear(in_features=128, out_features=10)
→ LogSoftMax()

After training, the final model has a 99% test accuracy. For most of the training samples, the predicted probabilities have a low entropy and are close to a one-hot vector. Consequently, the overall variance of the estimated FIM is very close to zero.

G.3 Evaluation

To compute the FIM, we only consider the weight and bias parameters in the first layer for simplicity. We randomly choose a fixed $x$ with multiple sampled $y_i$ for calculation, as per Eqs. (7) and (8). Recall that the randomness of our estimators comes from the sampling of $y_i \sim p(y \mid x)$. For all related computation, we use double-precision floating point (64 bits). The FIM estimations for both a trained model and a random model are given in Figs. A.2a and A.2b.

To calculate the “true” variance to compare against the bounds, we use Monte-Carlo estimation using a large number (1,000 for the presented results) of samples. Then, the variance of the estimator is approximated by the sample variance.

G.4 Results

We plot the histograms of the ratio of the estimated variance of $\hat{I}_1(\theta)$ ($\hat{I}_2(\theta)$) over the variance bound given by Theorem 7 (Theorem 8). For the trained network, the plot is given by Fig. A.3a (Fig. A.4a); for the random network, the plot is by Fig. A.3b (Fig. A.4b). In both the trained and random models, the bounds are empirically verified (the ratio is always smaller than 1). When comparing the ratio histograms, a smaller ratio value corresponds to a looser bound. We can immediately see that the trained network’s bounds are looser than that of the randomized network.

We also plot of the (Frobenius) distance $\|\hat{I}_1(\theta) - \hat{I}_2(\theta)\|_F$ between the two estimators over the number of samples for calculating the estimators. See Figs. A.5a and A.5b for the cases of trained and random networks, respectively. As the trained model has a very small variance of $y_i$, it is hard to observe in Fig. A.5a any change of the distance between $\hat{I}_1(\theta)$ and $\hat{I}_2(\theta)$ as the samples increase. For the randomized model, we do observe the decrease in estimator distance as the number of samples increase, as expected, Fig. A.5b.
H  Univariant Gaussian

We consider the case where we parameterize a univariant Gaussian distribution and consider the FIM and the corresponding estimators quantities.

Firstly, we specify Eq. (3) for a univariant Gaussian by setting:

\[ t(y) = (y, y^2); \quad F(h) = -\frac{h_1^2}{4h_2} + \frac{1}{2} \ln \left( \frac{-\pi}{h_2} \right), \]

where \( y = y \in \mathbb{R} \) and \( h = h_L \) for readability.

In particular, the 2 dimensional output neural network parametrizes the mean \( \mu \) and standard deviation \( s \) by:

\[ h = \left( \mu, \frac{-1}{2s^2} \right). \]

Furthermore, we have dual coordinates:

\[ \eta = \left( -\frac{h_1}{2h_2}, \frac{h_1^2 - 2h_2}{4h_2^2} \right) = (\mu, \mu^2 + s^2). \]

The closed form for the FIM/covariance matrix is given by:

\[ I(h) = \text{Var}(t) = \begin{bmatrix} -\frac{1}{2h_2} & \frac{h_1}{2h_2^2} \\ \frac{h_1}{2h_2^2} & -\frac{h_1^2}{4h_2^2} + \frac{1}{2h_2} \end{bmatrix}. \]

Notably, we have that \( h_1 \in \mathbb{R} \) and \( h_2 \in (-\infty, 0) \).

We present the following element-wise plots of FIM in Fig. A.6.

I  Residual Simple Cases

We look into the residual term which is present in the proof of Theorem 3. Specifically, the quantity:

\[ \mathcal{R}(\theta) = \int p(x) \frac{\partial^2}{\partial \theta \partial \theta} p(y \mid x) \, dy \, dx. \]

Consider the simple case where we only have a single weight and neuron,

\[ p(y \mid x) = \exp \left( t(y)h - F(h) \right), \quad h = \sigma(wx). \]

First consider the first derivative:

\[ \frac{\partial}{\partial w} p(y \mid x) = p(y \mid x) \cdot \frac{\partial}{\partial w} (t(y)h - F(h)) \]
\[ = p(y \mid x) \cdot (t(y) - \eta(h)) \cdot \sigma'(wx) \cdot x \]

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I.1 Assume that activation is identity

As \( \sigma'(z) = 1 \), we have the second derivative is the following:

\[
\frac{\partial^2}{\partial^2 w} p(y \mid x) = \frac{\partial}{\partial w} \left( p(y \mid x) \cdot (t(y) - \eta(h)) \cdot x \right)
\]

\[
= p(y \mid x) \left[ (t(y) - \eta(h))^2 \cdot x^2 - \nabla \eta(h) \cdot x^2 \right]
\]

Integrating the first term for the residual we have

\[
\int \int p(x)p(y \mid x) \cdot (t(y) - \eta(h))^2 \cdot x^2 \, dy \, dx = \int p(x) \cdot \nabla \eta(h) \cdot x^2 \, dx.
\]

Integrating the second term for the residual we have

\[
\int \int p(x)p(y \mid x) \cdot \nabla \eta(h) \cdot x^2 \, dy \, dx = \int p(x) \cdot \nabla \eta(h) \cdot x^2 \, dx.
\]

Thus by taking the difference, the residual is zero.

I.2 Assume that activation is not identity

The second derivative is the following:

\[
\frac{\partial^2}{\partial^2 w} p(y \mid x) = \frac{\partial}{\partial w} \left( p(y \mid x) \cdot (t(y) - \eta(h)) \cdot \sigma'(wx) \cdot x \right)
\]

\[
= \frac{\partial}{\partial w} \left( p(y \mid x) \right) \cdot (t(y) - \eta(h)) \cdot \sigma'(wx) \cdot x
\]

\[
+ p(y \mid x) \cdot \frac{\partial}{\partial w} \left( t(y) - \eta(h) \right) \cdot \sigma'(wx) \cdot x
\]

\[
+ p(y \mid x) \cdot (t(y) - \eta(h)) \cdot \frac{\partial}{\partial w} \left( \sigma'(wx) \right) \cdot x
\]

\[
= p(y \mid x) \cdot (t(y) - \eta(h))^2 \cdot \sigma'(wx)^2 \cdot x^2
\]

\[
+ p(y \mid x) \cdot (t(y) - \eta(h)) \cdot \sigma'(wx) \cdot x
\]

\[
+ p(y \mid x) \cdot (t(y) - \eta(h)) \cdot \frac{\partial}{\partial w} \left( \sigma'(wx) \right) \cdot x
\]

\[
= p(y \mid x) \cdot (t(y) - \eta(h))^2 \cdot \sigma'(wx)^2 \cdot x^2
\]

\[
- p(y \mid x) \cdot \nabla \eta(h) \cdot \sigma'(wx)^2 \cdot x^2
\]

\[
+ p(y \mid x) \cdot (t(y) - \eta(h)) \cdot \frac{\partial}{\partial w} \left( \sigma'(wx) \right) \cdot x.
\]

By the linearity of the integral, we calculate each term of the residual. For the first term:

\[
\int \int p(x) \cdot p(y \mid x) \cdot (t(y) - \eta(h))^2 \cdot \sigma'(wx)^2 \cdot x^2 \, dy \, dx
\]

\[
= \int p(x) \cdot \sigma'(wx)^2 \cdot x^2 \int p(y \mid x) \cdot (t(y) - \eta(h))^2 \, dy \, dx
\]

\[
= \int p(x) \cdot \sigma'(wx)^2 \cdot x^2 \cdot \nabla \eta(h) \, dx.
\]
Given that the second term only has \( p(y \mid x) \) which is dependent on \( y \), the first and second term of the residual cancel out. Thus we only have:

\[
R(w) = \int \int p(x)p(y \mid x) \cdot (t(y) - \eta(h)) \cdot \frac{\partial}{\partial w} (\sigma'(wx)) \cdot x \, dy \, dx
\]

\[
= \int \int p(x)p(y \mid x) \cdot \frac{\partial}{\partial w} (\sigma'(wx)) \cdot x \, dy \, dx
\]

\[
- \int \int p(x)p(y \mid x) \cdot \eta(h) \cdot \frac{\partial}{\partial w} (\sigma'(wx)) \cdot x \, dy \, dx
\]

\[
= \int p(x) \cdot \frac{\partial}{\partial w} (\sigma'(wx)) \cdot x \int p(y \mid x) \cdot t(y) \, dy \, dx - \int p(x) \cdot \eta(h) \cdot \frac{\partial}{\partial w} (\sigma'(wx)) \cdot x \, dx.
\]

Given that

\[
\frac{\partial}{\partial w} (\sigma'(wx)) = \delta(wx)
\]

and

\[
\int f(x)\delta(x) \, dx = f(0), \tag{A.12}
\]

the residual will result in zero for this case.
(a) $\hat{I}_1(\theta)$ and $\hat{I}_2(\theta)$, where $\theta$ is a random model. Color values are shared.

(b) $\tilde{I}_1(\theta)$ and $\tilde{I}_2(\theta)$, where $\theta$ is a trained model. Color values are shared.

Figure A.2: The estimated FIM presented in heatmaps corresponding to the first layer of a CNN.
Figure A.3: Ratio of the bound of the variance in Theorem 7 over the true estimated variance.

Figure A.4: Ratio of the bound of the variance in Theorem 8 over the true estimated variance.

Figure A.5: Distance between estimator $\hat{I}_1(\theta)$ and $\hat{I}_2(\theta)$. 
Figure A.6: Normal distribution $I(h)$. 

$$
\begin{array}{c}
\begin{array}{c}
\begin{array}{c}
I_{11}(h) \\
I_{12}(h) \text{ and } I_{21}(h) \\
I_{22}(h)
\end{array}
\end{array}
\end{array}
$$