A Geometric Modeling of Occam’s Razor in Deep Learning

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Abstract

Why do deep neural networks (DNNs) benefit from very high dimensional parameter spaces? Their huge parameter complexities vs. stunning performances in practice is all the more intriguing and not explainable using the standard theory of model selection for regular models. In this work, we propose a geometrically flavored information-theoretic approach to study this phenomenon. Namely, we introduce the locally varying dimensionality of the parameter space of neural network models by considering the number of significant dimensions of the Fisher information matrix, and model the parameter space as a manifold using the framework of singular semi-Riemannian geometry. We derive model complexity measures which yield short description lengths for deep neural network models based on their singularity analysis thus explaining the good performance of DNNs despite their large number of parameters.

1 Introduction

Deep neural networks (DNNs) are usually large models in terms of storage costs. In the classical model selection theory, such models are not favored as compared to simple models with the same training performance. For example, if one applies the Bayesian information criterion (BIC) [63] to DNN, a shallow neural network (NN) will be preferred over a deep NN due to the penalty term with respect to (w.r.t.) the complexity. A basic principle in science is the Occam’s Razor, which favors simple models over complex ones that accomplish the same task. This raises the fundamental question of how to measure the simplicity or the complexity of a model.

Formally, the preference of simple models has been studied in the area of minimum description length (MDL) [22, 59, 60], also known in another thread of research as the minimum message length (MML) [69].

*This work first appeared under the former title “Lightlike Neuromanifolds, Occam’s Razor and Deep Learning” in 2019.

1William of Ockham (ca. 1287 — ca. 1347), a monk (friar) and philosopher.
Consider a parametric family of distributions \( \mathcal{M} = \{ p(x \mid \theta) \} \) with \( \theta \in \Theta \subset \mathbb{R}^D \). The distributions are mutually absolutely continuous, which guarantees all densities to have the same support. Otherwise, many problems of non-regularity will arise as described by [24, 55]. The Fisher information matrix (FIM) \( \mathcal{I}(\theta) \) is a \( D \times D \) positive semi-definite (psd) matrix: \( \mathcal{I}(\theta) \succeq 0 \). The model is called regular if it is (i) identifiable [11] with (ii) a non-degenerate and finite Fisher information matrix (i.e., \( \mathcal{I}(\theta) \succ 0 \)).

In a Bayesian setting, the description length of a set of \( N \) i.i.d. observations \( X = \{ x_i \}_{i=1}^N \subset \mathcal{X} \) w.r.t. \( \mathcal{M} \) can be defined as the number of nats with the coding scheme of a parametric model \( p(x \mid \theta) \) and a prior \( p(\theta) \). The code length of any \( x_i \) is given by the cross entropy between the empirical distribution \( \delta_i(x) = \delta(x - x_i) \), where \( \delta(\cdot) \) denotes the Dirac’s delta function, and

\[
p(x) = \int p(x \mid \theta) p(\theta) \, d\theta.
\]

Therefore, the description length of \( X \) is

\[
- \log p(X) = \sum_{i=1}^N h^\times(\delta_i : p) = -\sum_{i=1}^N \log \int p(x_i \mid \theta) p(\theta) \, d\theta, 
\]

where \( h^\times(p : q) := -\int p(x) \log q(x) dx \) denotes the cross entropy between \( p(x) \) and \( q(x) \), and log denotes natural logarithm throughout the paper. The code length means the cumulative loss of the Bayesian mixture model \( p(x) \) w.r.t. the observations \( X \).

By using Jeffreys\(^2\) non-informative prior [3] as \( p(\theta) \), the MDL in eq. (1) can be approximated (see [7, 59, 60]) as

\[
\chi = \frac{\text{geometric complexity}}{\text{fitness}} + \frac{\text{penalize high dof}}{\text{model capacity}} = \log \left( \frac{\det(\mathcal{I}(\theta))}{\sqrt{|\theta|}} \right) - \frac{D}{2} \log \frac{N}{2\pi} + \log \left( \frac{D}{2} \log \frac{N}{2\pi} \right),
\]

where \( \hat{\theta} \in \Theta \) is the maximum likelihood estimation (MLE), or the projection [3] of \( X \) onto the model, \( D = \text{dim}(\Theta) \) is the model size, \( N \) is the number of observations, and \( | \cdot | \) denotes the matrix determinant. In this paper, the symbols \( \chi \) and \( O \) and the term “razor” all refer to the same concept, that is the description length of the data \( X \) by the model \( M \). The smaller those quantities, the better.

The first term in eq. (2) is the fitness of the model to the observed data. The second and the third terms measures the geometric complexity [44] and make \( \chi \) favor simple models. The second \( O(\log N) \) term only depends on the number of parameters \( D \) and the number of observations \( N \). It penalizes large models with a high degree of freedom (dof). The third \( O(1) \) term is independent to the observed data and measures the model capacity, or the total “number” of distinguishable distributions [44] in the model.

Unfortunately, this razor \( \chi \) in eq. (2) does not fit straightforwardly into DNNs, which are high-dimensional singular models. The FIM \( \mathcal{I}(\theta) \) are large singular matrices (not full rank) and the last term may be difficult to evaluate. Based on the second term on the right-hand-side (RHS), a DNN can have very high complexity and therefore is less favored against a shallow network. This contradicts the good generalization of DNNs as compared to shallow NNs. These issues call for a new analysis of the MDL in the DNN setting.

Towards this direction, we made the following contributions in this paper:

- New concepts and methodologies from singular semi-Riemannian geometry [36] to analyze the space of neural networks;

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\(^2\)Sir Harold Jeffreys (1891–1989), a British statistician.
- A definition of the local dimensionality, that is the amount of non-singularity, with bounding analysis;
- A new MDL formulation, which explains how the singularity contribute to the “negative complexity” of DNNs: That is, the model turns simpler as the number of parameters grows.

The rest of this paper is organized as follows. Section 2 reviews singularities in information geometry. In the setting of a DNN, section 3 introduces its singular parameter manifold. Section 4 bounds the number of singular dimensions of the parameter manifold of the DNN. Sections 5 to 8 derive our MDL criterion based on two different priors, and discusses how model complexity is affected by the singular geometry. We discuss related work in section 9 and conclude in section 10.

2 Lightlike Statistical Manifold

In this paper, bold capital letters like $A$ denote matrices, bold small letters like $a$ denote vectors, normal capital/small letters like $A/a$ and Greek letters like $\alpha$ denote scalars, and calligraphy letters like $M$ denote manifolds (with exceptions).

The term “statistical manifold” refers to $\mathcal{M} = \{ p(x | \theta) \}$, where each point of $\mathcal{M}$ corresponds to a probability distribution $p(x | \theta)$. The discipline of information geometry [3] studies such a space in the Riemannian and more generally differential geometry framework. Hotelling [26] and independently Rao [57, 58] proposed to endow a parametric space of statistical models with the Fisher information matrix as a Riemannian metric:

$$ I(\theta) := \mathbb{E}_p \left( \frac{\partial \log p(x | \theta)}{\partial \theta} \frac{\partial \log p(x | \theta)}{\partial \theta^\intercal} \right), $$

where $\mathbb{E}_p$ denotes the expectation w.r.t. $p(x | \theta)$. The corresponding infinitesimal squared length element $ds^2 = \text{tr}(I(\theta)d\theta d\theta^\intercal) = \langle d\theta, d\theta \rangle_{I(\theta)} = d\theta^\intercal I(\theta) d\theta$, where $\text{tr}(\cdot)$ means the matrix trace, is independent of the underlying parameterization of the population space.

Amari further developed this approach by revealing the dualistic structure of statistical manifolds which extends the Riemannian framework [3, 48]. The MDL criterion arising from the geometry of Bayesian inference with Jeffreys’ prior for regular models is detailed in [7]. In information geometry, the regular assumption is (1) an open connected parameter space in some Euclidean space; and (2) the FIM exists and is non-singular. However, in general, the FIM is only positive semi-definite and thus for non-regular models like neuromanifolds [3] or Gaussian mixture models [70], the manifold is not Riemannian but singular semi-Riemannian [15, 36]. In the machine learning community, singularities have often been dealt with as a minor issue: For example, the natural gradient has been generalized based on the Moore-Penrose inverse of $I(\theta)$ [67] to avoid potential non-invertible FIMs. Watanabe [70] addressed the fact that most usual learning machines are singular in his singular learning theory which relies on algebraic geometry. Nakajima and Ohmoto [46] discussed dually flat structures for singular models.

Recently, preliminary efforts [6, 28] tackle singularity at the core, mostly from a mathematical standpoint. For example, Jain et al. [28] studied the Ricci curvature tensor of such manifolds. These mathematical notions are used in the community of differential geometry or general relativity but have not yet been ported to the machine learning community.

Following these efforts, we first introduce informally some basic concepts from a machine learning perspective to define the differential geometry of non-regular statistical manifolds. The

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3To be more precise, a statistical manifold [37] is a structure $(\nabla, g, C)$ on a smooth manifold $\mathcal{M}$, where $g$ is a metric tensor, $\nabla$ a torsion-free affine connection, and $C$ is a symmetric covariant tensor of order 3.

4Using the cyclic property of the matrix trace, we have $ds^2 = \text{tr}(I(\theta)d\theta d\theta^\intercal) = d\theta^\intercal I(\theta) d\theta$. 

3
a null curve
(equivalent models)

Figure 1: A toy lightlike manifold \( \mathcal{M} \) with a null curve. The ellipses are Tissot’s indicatrices, showing how circles of infinitesimal radius are distorted by the lightlike geometry on \( \mathcal{M} \). On the null curve, the FIM is degenerate so that \( \langle \partial \theta_i, \partial \theta_i \rangle_I = 0 \). Therefore the local dynamic \( \partial \theta_i \) (tangent vector of the null curve) has zero length, meaning that it does not change the model. The radical distribution \( \text{Rad}(T \mathcal{M}) \) is formed by the null curve and its tangent vectors.

tangent space \( T_\theta(\mathcal{M}) \) is a \( D \)-dimensional \( (D = \dim(\mathcal{M})) \) real vector space, that is the local linear approximation of the manifold \( \mathcal{M} \) at the point \( \theta \in \mathcal{M} \), equipped with the inner product induced by \( I(\theta) \). The tangent bundle \( T \mathcal{M} := \{(\theta, v), \theta \in \mathcal{M}, v \in T_\theta \} \) is the 2\( D \)-dimensional manifold obtained by combining all tangent spaces for all \( \theta \in \mathcal{M} \). A vector field is a smooth mapping from \( \mathcal{M} \) to \( T \mathcal{M} \) such that each point \( \theta \in \mathcal{M} \) is attached a tangent vector originating from itself. Vector fields are cross-sections of the tangent bundle. In a local coordinate chart \( \theta \), the vector fields along the frame are denoted as \( \partial \theta_i \). A distribution (not to be confused with probability distributions which are points on \( \mathcal{M} \)) means a vector subspace of the tangent bundle spanned by several independent vector fields, such that each point \( \theta \in \mathcal{M} \) is associated with a subspace of \( T_\theta(\mathcal{M}) \) and those subspaces vary smoothly with \( \theta \). Its dimensionality is defined by the dimensionality of the subspace, i.e., the number of vector fields that span the distribution.

In a lightlike manifold \cite{15, 36} \( \mathcal{M}, I(\theta) \) can be degenerate. The tangent space \( T_\theta(\mathcal{M}) \) is a vector space with a kernel subspace, i.e., a nullspace. A null vector field is formed by null vectors, whose lengths measured according to the Fisher metric tensor are all zero. The radical distribution \( \text{Rad}(T \mathcal{M}) \) is the distribution spanned by the null vector fields. Locally at \( \theta \in \mathcal{M} \), the tangent vectors in \( T_\theta(\mathcal{M}) \) which span the kernel of \( I(\theta) \) are denoted as \( \text{Rad}_\theta(T \mathcal{M}) \). In a local coordinate chart, \( \text{Rad}(T \mathcal{M}) \) is well defined if these \( \text{Rad}_\theta(T \mathcal{M}) \) form a valid distribution. We write \( T \mathcal{M} = \text{Rad}(T \mathcal{M}) \oplus \mathcal{S}(T \mathcal{M}) \), where “\( \oplus \)” is the direct sum, and the screen distribution \( \mathcal{S}(T \mathcal{M}) \) is complementary to the radical distribution \( \text{Rad}(T \mathcal{M}) \) and has a non-degenerate induced metric. See fig. 1 for an illustration of the concept of radical distribution.

We can find a local coordinate frame (a frame is an ordered basis) \( \{\theta_1, \ldots, \theta_d, \theta_{d+1}, \ldots, \theta_D\} \), where the first \( d \) dimensions \( \theta^* = (\theta_1, \ldots, \theta_d) \) correspond to the screen distribution, and the remaining \( d := D - d \) dimensions \( \theta^\prime = (\theta_{d+1}, \ldots, \theta_D) \) correspond to the radical distribution. The

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Radical stems from Latin and means root.
local inner product $\langle \cdot , \cdot \rangle_I$ satisfies
\[
\langle \partial \theta_i, \partial \theta_j \rangle_I = \delta_{ij}, \quad (\forall \ 1 \leq i, j \leq d)
\]
\[
\langle \partial \theta_i, \partial \theta_k \rangle_I = 0, \quad (\forall \ d + 1 \leq i \leq D, \ 1 \leq k \leq D)
\]
where $\delta_{ij} = 1$ if and only if (iff) $i = j$ and $\delta_{ij} = 0$, otherwise. Unfortunately, this frame is not unique [14]. We will abuse $I$ to denote both the FIM of $\theta$ and the FIM of $\theta^*$. One has to remember that $I(\theta) \succeq 0$, while $I(\theta^*) \succ 0$ is a proper Riemannian metric. Hence, both $I^{-1}(\theta^*)$ and $\log |I(\theta^*)|$ are well-defined.

Remark 1. Notice that the Fisher information matrix is covariant under reparameterization. That is, let $\theta(\lambda)$ be an invertible smooth reparameterization of $\lambda$. Then the FIM rewrites in the $\theta$-parameterization as:
\[
I(\theta) = J_{\theta \to \lambda}^T I(\lambda(\theta)) J_{\theta \to \lambda},
\]
where $J_{\theta \to \lambda}$ is the full rank Jacobian matrix.

The natural gradient flows (vector fields on $M$) with respect to $\lambda$ and $\theta$ coincide but not the natural gradient descent methods (learning paths that consist of sequences of points on $M$) because of the non-zero learning step sizes.

Furthermore, the ranks of $I(\theta)$ and $I(\lambda)$ as well as the dimensions of the screen and radical distributions coincide. Hence, the notion of singularities is intrinsic and independent of the smooth reparameterization.

3 Lightlike Neuromanifold

This section instantiates the concepts in the previous section 2 in terms of a simple DNN predictive model. The random variable $x = (z, y)$ of interest consists of two components: $z$, referred to as the “input”, and $y$, referred to as the “target”. By assumption, their joint probability distribution is specified by
\[
\log p(x | \psi, \theta) = \log p(z | \psi) + \log p(y | z, \theta),
\]
where $p(z | \psi)$ is a generative model of $z$ which is parameterized by $\psi$, $p(y | z, \theta)$ is a predictive DNN, and $\theta$ consists of all neural network parameters.

Our main subject is the latter predictive model $p(y | z, \theta)$ and its parameter manifold $M_\theta$. Here, we need the generative model $p(z | \psi)$ for the purpose of discussing how the geometry of $M_\theta$ is affected by the choice of $p(z | \psi)$ and can be studied independent of the parameter space of $p(z | \psi)$, which we denote as $M_\psi$. In the end, our results do not depend on the specific form of $p(z)$ or whether it is parametric.

For $p(y | z, \theta)$, we consider a deep feed-forward network with $L$ layers, uniform width $M$ except the last layer which has $m$ output units ($m < M$), input $z \in Z$ with $\dim(Z) = M$, pre-activations $h^l$ of size $M$ (except that in the last layer, $h^L$ has $m$ elements), post-activations $z^l$ of size $M$, weight matrices $W^l$ and bias vectors $b^l$ ($1 \leq l \leq L$). The layers are given by
\[
\begin{align*}
  z^l &= \phi(h^l), \\
  h^l &= W^l z^{l-1} + b^l, \\
  z^0 &= z,
\end{align*}
\]
where $\phi$ is an element-wise nonlinear activation function such as ReLU [19].
Without loss of generality, we assume multinomial\(^\text{6}\) output units and the DNN output \([20]\)

\[ y \sim \text{Multinomial} \left( \text{SoftMax}(h^L) \right) \]

is a random label in the set \(\{1, \cdots, m\}\), where

\[ \text{SoftMax}(t) := \frac{1}{\sum_{i=1}^{m} \exp(t_i)} (\exp(t_1), \exp(t_2), \cdots, \exp(t_m)) \]

denotes the softmax function. \(\text{SoftMax}(h^L)\) is a random point in \(\Delta^m\), the \((m-1)\) dimensional statistical simplex. Therefore, \(p(y = k) = \exp(h^L_k)/\sum_{j=1}^{m} \exp(h^L_j)\), \(k = 1, \cdots, m\). The neural network parameters \(\theta\) consists of \(W\) and \(b\), \(l = 1, \cdots, L\). In this supervised setting, the code length in eq. (1) means the predictive loss of the Bayesian mixture model \(p(x) = p(z) \int p(y | z, \theta)p(\theta) d\theta\) w.r.t. to the observed pairs \((z_i, y_i)\). The smaller the code length, the more accurate the prediction.

All such neural networks \(\text{NN}_\theta\) when \(\theta\) varies in a parameter space are referred to as the neuromapifold: \(\mathcal{M}_\theta = \{ \text{NN}_\theta : \theta \in \Theta\} \). Similarly, the parameter space of the distribution family \(p(z | \psi)\) is denoted as \(\mathcal{M}_\psi\). In machine learning, we are often interested in the FIM w.r.t. \(\theta\) as it reveals the geometry of the parameter space. However, the FIM can also be computed relatively w.r.t. a subset of \(\theta\) in a sub-system \([65]\).

By the definition in eq. (3), the FIM on the product manifold \(\mathcal{M}_\psi \times \mathcal{M}_\theta\) is in a block-diagonal form

\[ \mathcal{I}(\psi, \theta) = \begin{bmatrix} \mathcal{I}(\psi) & 0 \\ 0 & \mathcal{I}(\theta) \end{bmatrix}. \tag{6} \]

The off-diagonal block is zero-matrix (denoted as \(0\)) because

\[
\begin{align*}
\mathbb{E}_p \left( \frac{\partial \log p(x | \psi, \theta)}{\partial \psi} \frac{\partial \log p(x | \psi, \theta)}{\partial \theta^\top} \right) &= \mathbb{E}_p \left( \frac{\partial \log p(z | \psi)}{\partial \psi} \frac{\partial \log p(y | z, \theta)}{\partial \theta^\top} \right) \\
&= \mathbb{E}_{p(z|\psi)} \left( \frac{\partial \log p(z | \psi)}{\partial \psi} \mathbb{E}_{p(y|z, \theta)} \left( \frac{\partial \log p(y | z, \theta)}{\partial \theta} \right)^\top \right) = 0,
\end{align*}
\]

where \(\mathbb{E}_{p(y|z, \theta)} \left( \frac{\partial \log p(y|z, \theta)}{\partial \theta} \right)\) is the expectation of the score function and is always zero. The metric \(\mathcal{I}(\psi, \theta)\) is a product metric, meaning that the geometry of \(\mathcal{M}_\theta\) defined by \(\mathcal{I}(\theta)\) can be studied separately to the geometry of \(\mathcal{M}_\psi\).

As we are interested in the predictive model corresponding to the diagonal block \(\mathcal{I}(\theta)\), we further have (see e.g. \([51],[64]\) for derivations)

\[ \mathcal{I}(\theta) = \mathbb{E}_p(z) \left[ \left( \frac{\partial h^L(z)}{\partial \theta} \right)^\top C(z) \frac{\partial h^L(z)}{\partial \theta} \right], \tag{7} \]

where the expectation is taken w.r.t. \(p(z) := p(z | \psi)\), an underlying true distribution in the input space depending on the parameter \(\psi\). \(\frac{\partial h^L(z)}{\partial \theta}\) is the \(m \times D\) parameter-output Jacobian matrix, based on a given input \(z\), \(C(z) := \text{diag}(o(z)) - o(z)o(z)^\top \succeq 0\), \(\text{diag}(\cdot)\) means the diagonal matrix with the given diagonal entries, and \(o(z) := \text{SoftMax}(h^L(z))\) is the predicted class probabilities of \(z\). By the definition of SoftMax, each dimension of \(o(z)\) represents a positive probability, although \(o(z)\) can be arbitrarily close to a one-hot vector. As a result, the kernel of

\[ \text{SoftMax}(t) := \frac{1}{\sum_{i=1}^{m} \exp(t_i)} (\exp(t_1), \exp(t_2), \cdots, \exp(t_m)) \]

\[ y \sim \text{Multinomial} \left( \text{SoftMax}(h^L) \right) \]

\[ \text{SoftMax}(t) := \frac{1}{\sum_{i=1}^{m} \exp(t_i)} (\exp(t_1), \exp(t_2), \cdots, \exp(t_m)) \]

\[ y \sim \text{Multinomial} \left( \text{SoftMax}(h^L) \right) \]

\[ \text{SoftMax}(t) := \frac{1}{\sum_{i=1}^{m} \exp(t_i)} (\exp(t_1), \exp(t_2), \cdots, \exp(t_m)) \]

\[ y \sim \text{Multinomial} \left( \text{SoftMax}(h^L) \right) \]
the psd matrix $C(z)$ is given by $\{\lambda 1 : \lambda \in \mathbb{R}\}$, where 1 is the vector of all 1’s. See our analysis in appendix B.

In eq. (7), $\mathcal{I}(\theta)$ is the single-observation FIM. It is obvious that the FIM w.r.t. the joint distribution $p(X \mid \theta)$ of multiple observations is $N \mathcal{I}(\theta)$ (Fisher information is additive), so that $\mathcal{I}(\theta)$ does not scale with $N$. Notice that we use $X$, $Y$ and $Z$ to denote a collection of $N$ random observations and use $x$, $y$ and $z$ to denote one single observation.

In general, to compute $\mathcal{I}(\theta)$ needs to assume $p(z)$, which depends on the parameter $\psi$. This makes sense as $(\psi_1, \theta)$ and $(\psi_2, \theta)$ with $\psi_1 \neq \psi_2$ are different points on the product manifold $\mathcal{M}_\phi \times \mathcal{M}_\theta$ and thus their $\mathcal{I}(\theta)$ should be different. In practice, one only gets access to a set of $N$ i.i.d. samples drawn from an unknown $p(z \mid \psi)$. In this case, it is reasonable to take $p(z)$ in eq. (7) to be the empirical distribution $\hat{p}(z)$ so that $p(z) = \hat{p}(z) := \frac{1}{N} \sum_{i=1}^{N} \delta(z - z_i)$, then

$$\mathcal{I}(\theta) = \hat{\mathcal{I}}(\theta) := \frac{1}{N} \sum_{i=1}^{N} \left[ \left( \frac{\partial h^L(z_i)}{\partial \theta} \right)^\top C(z_i) \frac{\partial h^L(z_i)}{\partial \theta} \right].$$

(8)

In fact, one can skip assuming a generative model $p(z \mid \psi)$ and choosing a $\psi$. $\hat{\mathcal{I}}(\theta)$ can be directly computed from the observed $z_i$’s and does not depend on the observed $y_i$’s. Although denoted differently than $\mathcal{I}(\theta)$ in the current paper, this $\hat{\mathcal{I}}(\theta)$ is a standard version of the definition of the FIM for neural networks [35, 42, 64, 65].

By considering the neural network weights and biases as random variables satisfying a prescribed prior distribution [30, 54], this $\mathcal{I}(\theta)$ can be regarded as a random matrix [43] depending on the structure of the DNN and the prior. The empirical density of $\mathcal{I}(\theta)$ is the empirical distribution of its eigenvalues $\{\lambda_i\}_{i=1}^{D}$, that is, $\rho_D(\lambda) = \frac{1}{D} \sum_{i=1}^{D} \delta(\lambda_i)$. If at the limit $D \to \infty$, the empirical density converges to a probability density function (pdf), then

$$\rho_{\mathcal{I}}(\lambda) := \lim_{D \to \infty} \rho_D(\lambda)$$

(9)

is called the spectral density of the Fisher information matrix.

For DNN, we assume that

(A1) At the MLE $\hat{\theta}$, the prediction SoftMax($h^L(z_i)$) perfectly recovers (tending to be one-hot vectors) the training target $y_i$, for all the training samples $(z_i, y_i)$.

In this case, the negative Hessian of the average log-likelihood

$$\mathcal{J}(\theta) := -\frac{1}{N} \frac{\partial^2 \log p(X \mid \theta)}{\partial \theta \partial \theta^\top} = -\frac{1}{N} \sum_{i=1}^{N} \frac{\partial^2 \log p(y_i \mid z_i, \theta)}{\partial \theta \partial \theta^\top}$$

is called the observed FIM (sample-based FIM), which is also known as the “empirical Fisher” in machine learning literature [35, 42]. In our notations explained in table 1, the FIM $\mathcal{I}$ depends on the true distribution $p(z)$ and does not depend on the observed samples. In the expression of the FIM in eq. (7), if $p(z) = \hat{p}(z)$, then $\mathcal{I}$ become $\hat{\mathcal{I}}$, which depends on the observed input $z_i$’s. The observed FIM $\mathcal{J}$ depends on both the observed input $z_i$’s and the observed target $y_i$’s. If $p(z) = \hat{p}(z)$, the observed FIM coincides with the FIM at the MLE $\hat{\theta}$ and $\mathcal{J}(\theta) = \hat{\mathcal{I}}(\theta)$. For general statistical models, there is a residual term in between these two matrices which scales with the training error (see e.g. Eq. 6.19 in section 6 of [4], or eq. (20) in the appendix). How these different metric tensors are called is just a matter of terminology. One should distinguish them by examining whether/how they depend (partially) on the observed information.
Table 1: The FIM and the observed FIM. The last three columns explains whether the tensor depends on the observed $z_i$’s, whether it depends on the observed $y_i$’s, and whether they can be computed in practice.

| Notation | Name                          | Depend on $z_i$ | Depend on $y_i$ | Computable |
|----------|-------------------------------|----------------|----------------|------------|
| $\mathcal{I}(\theta)$ | FIM (w.r.t. true $p(z)$)       | No             | No             | No         |
| $\hat{\mathcal{I}}(\theta)$ | FIM (w.r.t. empirical $\hat{p}(z)$) | Yes            | No             | Yes        |
| $\mathfrak{J}(\theta)$ | observed FIM                  | Yes            | Yes            | Yes        |

4 Local Dimensionality

This section quantitatively measures the singularity of the neuromanifold. Our main definitions and results do not depend on the settings introduced in the previous section and can be generalized to similar models including stochastic neural networks [10]. For example, if the output units or the network structure is changed, the expression of the FIM and related results can be adapted straightforwardly. Our derivations depend on that (1) DNNs have a large amount of singularity corresponding zero eigenvalues of the FIM; and (2) the spectrum of the (observed) FIM has many eigenvalues close to zero [31]. That being said, our results also apply to singular models [70] with similar properties.

Definition 1 (Local dimensionality). The local dimensionality $d(\theta) := \text{rank}(\mathcal{I}(\theta))$ of the neuromanifold $\mathcal{M}$ at $\theta \in \mathcal{M}$ refers to the rank of the FIM $\mathcal{I}(\theta)$. If $p(z) = \hat{p}(z)$, then $d(\theta) = \hat{d}(\theta) := \text{rank}(\hat{\mathcal{I}}(\theta))$.

The local dimensionality $d(\theta)$ is the number of degrees of freedom at $\theta \in \mathcal{M}$ which can change the probabilistic model $p(y|z, \theta)$ in terms of information theory. One can find a reparameterized DNN with $d(\theta)$ parameters, which is locally equivalent to the original DNN with $D$ parameters. Recall the dimensionality of the tangent bundle is two times the dimensionality of the manifold.

Remark 2. The dimensionality of the screen distribution $S(\mathcal{T}\mathcal{M})$ at $\theta$ is $2d(\theta)$.

By definition, the FIM as the singular semi-Riemannian metric of $\mathcal{M}$ must be psd. Therefore it only has positive and zero eigenvalues, and the number of positive eigenvalues $d(\theta)$ is not constant as $\theta$ varies in general.

Remark 3. The local metric signature (number of positive, negative, zero eigenvalues of the FIM) of the neuromanifold $\mathcal{M}$ is $(d(\theta), 0, D - d(\theta))$, where $d(\theta)$ is the local dimensionality.

The local dimensionality $d(\theta)$ depends on the specific choice of $p(z)$. If $p(z) = \hat{p}(z)$, then $d(\theta) = \hat{d}(\theta) = \text{rank}(\hat{\mathcal{I}}(\theta))$. On the other hand, one can use the rank of the negative Hessian $\mathfrak{J}(\theta)$ (i.e., observed rank) to get an approximation of the local dimensionality $d(\theta) \approx \text{rank}(\mathfrak{J}(\theta))$. In the MLE $\hat{\theta}$, this approximation becomes accurate. We simply denote $d$ and $\hat{d}$, instead of $d(\theta)$ and $\hat{d}(\theta)$, if $\theta$ is clear from the context.

We first show that the lightlike dimensions of $\mathcal{M}$ do not affect the neural network model in eq. (5).

Lemma 1. If $(\theta, \sum_j \alpha_j \partial \theta_j) \in \text{Rad}(\mathcal{T}\mathcal{M})$, i.e. $\langle \sum_j \alpha_j \partial \theta_j, \sum_j \alpha_j \partial \theta_j \rangle \mathcal{I}(\theta) = 0$, then almost surely we have $\frac{\partial h^k(z)}{\partial y} \alpha = \lambda(z)1$, where $\lambda(z) \in \mathbb{R}$, and $1$ is a vector of ones.
By lemma 1, the Jacobian $\frac{\partial h^L(z)}{\partial \theta}$ is the local linear approximation of the map $\theta \rightarrow h^L$. The dynamic $\alpha$ (coordinates of a tangent vector) on $\mathcal{M}$ causes a uniform increment on the output $h^L$, which, after the SoftMax function, does not change the neural network map $z \rightarrow y$.

Then, we have the following bounds.

**Proposition 2.** \( \forall \theta \in \mathcal{M}, d(\theta) \leq \min(D, (m - 1)N) \).

**Remark 4.** While the total number $D$ of free parameters is unbounded in DNNs, the local dimensionality estimated by $\hat{d}(\theta)$ grows at most linearly w.r.t. the sample size $N$, given fixed $m$ (size of the last layer). If both $N$ and $m$ are fixed, then $\hat{d}(\theta)$ is bounded even when the network width $M \rightarrow \infty$ and/or depth $L \rightarrow \infty$.

To understand $d(\theta)$, one can parameterize the DNN, locally, with only $d(\theta)$ free parameters while maintaining the same predictive model. The log-likelihood is a function of these $d(\theta)$ parameters, and therefore its Hessian has at most rank $d(\theta)$. In theory, one can only reparameterize $\mathcal{M}$ so that at one single point $\hat{\theta}$, the screen and radical distributions are separated based on the coordinate chart. Such a chart may neither exist locally (in a neighborhood around $\hat{\theta}$) nor globally.

The local dimensionality is not constant and may vary with $\theta$. The global topology of the neuromanifold is therefore like a stratifold [5, 16]. As $\theta$ has a large dimensionality in DNNs, singularities are more likely to occur in $\mathcal{M}$. Compared to the notion of intrinsic dimensionality [38], our $d(\theta)$ is well-defined mathematically rather than based on empirical evaluations. One can regard our local dimensionality as an upper bound of the intrinsic dimensionality, because a very small singular value of $\mathcal{I}$ still counts towards the local dimensionality. Notice that random matrices have full rank with probability 1 [17].

We can regard small singular values (below a prescribed threshold $\varepsilon > 0$) as $\varepsilon$-singular dimensions, and use $\varepsilon$-rank defined below to estimate the local dimensionality.

**Definition 2.** The $\varepsilon$-rank of the FIM $\mathcal{I}(\theta)$ is the number of eigenvalues of $\mathcal{I}(\theta)$ which is not less than some given $\varepsilon > 0$.

By definition, the $\varepsilon$-rank is a lower bound of the rank of the FIM, which depends on the $\theta$-parameterization — different parameterizations of the DNN may yield different $\varepsilon$-ranks of the corresponding FIM. If $\varepsilon \rightarrow 0$, the $\varepsilon$-rank of $\mathcal{I}(\theta)$ becomes the true rank of $\mathcal{I}(\theta)$ given by $d(\theta)$. The spectral density $p_{\varepsilon}$ (probability distribution of the eigenvalues of $\mathcal{I}(\theta)$) affects the $\varepsilon$-rank of $\mathcal{I}(\theta)$ and the expected local dimensionality of $\mathcal{M}$. On the support of $p_{\varepsilon}$, the higher the probability of the region $[0, \varepsilon]$, the more likely $\mathcal{M}$ is singular. By the Cramér-Rao lower bound, the variance of an unbiased 1D estimator $\hat{\theta}$ must satisfy

$$\text{var}(\hat{\theta}) \geq \mathcal{I}(\theta)^{-1} \geq \frac{1}{\varepsilon}.$$  

Therefore the $\varepsilon$-singular dimensions lead to a large variance of the estimator $\hat{\theta}$: a single observation $x_i$ carries little or no information regarding $\theta$, and it requires a large number of observations to achieve the same precision. The notion of thresholding eigenvalues close to zero may depend on the parameterization but the intrinsic ranks given by the local dimensionality are invariant.

In a DNN, there are several typical sources of singularities:

- First, if the neuron is saturated and gives constant output regardless of the input sample $z_i$, then all dynamics of its input and output connections are in $\text{Rad}(T, \mathcal{M})$.
- Second, two neurons in the same layer can have linearly dependent output, e.g. when they share the same weight vector and bias. They can be merged into one single neuron, as there exists redundancy in the original reparametrization.
• Third, if the activation function $\phi(\cdot)$ is homogeneous, e.g., ReLU, then any neuron in the DNN induces a reparametrization by multiplying the input links by $\alpha$ and output links by $1/\alpha^k$ ($k$ is the degree of homogeneity). This reparametrization corresponds to a null curve in the neuromanifold parameterized by $\alpha$.

• Fourth, certain structures such as recurrent neural networks (RNNs) suffer from vanishing gradient [20]. As the FIM is the variance of the gradient of the log-likelihood (known as variance of the score in statistics), its scale goes to zero along the dimensions associated with such structures.

It is meaningful to formally define the notion of “lightlike neuromanifold”. Using the geometric tools, related studies can be invariant w.r.t. neural network reparametrization. Moreover, the connection between neuromanifold and singular semi-Riemannian geometry, which is used in general relativity, is not yet widely adopted in machine learning. For example, the textbook [70] in singular statistics mainly used tools from algebraic geometry which is a different field.

Notice that the Fisher-Rao distance along a null curve is undefined because there the FIM is degenerate and there is no arc-length reparameterization along null curves [32].

5 General Formulation of Our Razor

In this section, we derive a new formula of MDL for DNNs, aiming to explain how does the high dimensional DNN structure can have a short code length of the given data? Notice that, this work focuses on the concept of model complexity but not the generalization bounds. We try to argue the DNN model is intrinsically simple because it can be described shortly. The theoretical connection between generalization power and MDL is studied in PAC-Bayesian theory and PAC-MDL (see [21, 25, 47] and references therein). This is beyond the scope of this paper.

We derive a simple asymptotic formula for the case of large sample size and large network size. Therefore crude approximations are taken and the low-order terms are ignored, which are common practices in deriving information criteria [1, 63].

In the following, we will abuse $p(x | \theta)$ to denote the DNN model $p(y | z, \theta)$ for shorter equations and to be consistent with the introduction. Assume

(A2) The absolute values of the third-order derivatives of $\log p(x | \theta)$ w.r.t. $\theta$ are bounded by some constant.

(A3) $\forall i, |\theta_i - \tilde{\theta}_i| = O(1/\sqrt{M})$, where $O(\cdot)$ is the Bachmann–Landau’s big-O notation.

Recall that $M$ is the width of the neural network. We consider that the neural networks weights have a order of $O(1/\sqrt{M})$. For example, if the input of a neuron follows the standard Gaussian distribution, then its weights with order $O(1/\sqrt{M})$ guarantee the output is $O(1)$. In practice, this constraint can be guaranteed by clipping the weight vector to a prescribed range.

We rewrite the code length in eq. (1) based on the Taylor expansion of $\log p(X | \theta)$ at $\theta = \hat{\theta}$ up to the second order:

\[
-\log p(X) = -\log \int_M p(\theta) \exp \left( \log p(X | \hat{\theta}) - \frac{N}{2} (\theta - \hat{\theta})^T \gamma(\hat{\theta})(\theta - \hat{\theta}) \right) d\theta + O \left( N\|\theta - \hat{\theta}\|^3 \right).
\]

Notice that the first order term vanishes because $\hat{\theta}$ is a local optimum of $\log p(X | \theta)$, and in the second order term, $-N\gamma(\hat{\theta})$ is the Hessian matrix of the likelihood function $\log p(X | \theta)$ evaluated
where \( \mu \)

Where \(" \) stands for Occam’s razor. Compared with previous formulations of MDL [7, 59, 60], eq. (12) relies on a quadratic approximation of the log-likelihood function and can be instantiated

The model has low complexity when there are many distributions on model capacity w.r.t. the prior and the capacity w.r.t. the posterior. A large log-ratio means

\( p(X|\theta) \propto p(\theta)p(X|\theta) \propto \kappa(\theta) \exp \left( -\frac{N}{2}(\theta - \hat{\theta})^\top \hat{\gamma}(\theta - \hat{\theta}) \right) \). It shrinks to zero when the number \( N \) of observations increases. The last two terms in eq. (12) is the log-ratio between the model capacity w.r.t. the prior and the capacity w.r.t. the posterior. A large log-ratio means there are many distributions on \( M \) which have a relatively large value of \( \kappa(\theta) \) but a small value of \( \kappa(\theta) \exp \left( -\frac{N}{2}(\theta - \hat{\theta})^\top \hat{\gamma}(\theta - \hat{\theta}) \right) \). The associated model is considered to have a high complexity, meaning that only a small “percentage” of the models are helpful to describe the given data.

DNNs have a large amount of symmetry: the parameter space consists many pieces that looks exactly the same. This can be caused e.g. by permutate the neurons in the same layer. This
is a different non-local property than singularity that is a local differential property. Our \( \mathcal{O} \) is not affected by the model size caused by symmetry, because these symmetric models are both counted in the prior and the posterior, and the log-ratio in eq. (12) cancels out symmetric models. Formally, \( \mathcal{M} \) has \( \zeta \) symmetric pieces denoted by \( \mathcal{M}_1, \ldots, \mathcal{M}_\zeta \). Note any MLE on \( \mathcal{M}_i \) is mirrored on those \( \zeta \) pieces. Then both integrations on the RHS of eq. (12) are multiplied by a factor of \( \zeta \). Therefore \( \mathcal{O} \) is invariant to symmetry.

6 Connection with f-mean

**Definition 3.** Given a set \( \mathcal{X} = \{t_i\}_{i=1}^n \subset \mathbb{R} \) and a continuous and strictly monotonous function \( f : \mathbb{R} \to \mathbb{R} \), the f-mean of \( \mathcal{X} \) is

\[
M_f(\mathcal{X}) := f^{-1} \left( \frac{1}{n} \sum_{i=1}^n f(t_i) \right).
\]

The f-mean, also known as the quasi-arithmetic mean was studied in [33, 45]: Thus they are also-called Kolmogorov-Nagumo means [34]. By definition, the image of \( M_f(\mathcal{X}) \) under \( f \) is the arithmetic mean of the image of \( \mathcal{X} \) under the same mapping. Therefore, \( M_f(\mathcal{X}) \) is in between the smallest and largest elements of \( \mathcal{X} \). If \( f(x) = x \), then \( M_f \) becomes the arithmetic mean, which we denote as \( \overline{x} \). We have the following bound.

**Lemma 4.** Given a real matrix \( T = (t_{ij})_{n \times m} \), we use \( t_i \) to denote \( i \)'th row of \( T \), and \( t_{.j} \) to denote the \( j \)'th column of \( T \). If \( f = \exp(-t) \), then

\[
M_f(T) \leq \{ M_f(t_{.1}), \ldots, M_f(t_{.m}) \} \leq M_f(\{\mathbf{1}_1, \ldots, \mathbf{1}_n\}) \leq T,
\]

where \( M_f(T) \) is the f-mean of all \( n \times m \) elements of \( T \), and \( T \) is their arithmetic mean.

In the above inequality, if the arithmetic mean of each row is first evaluated, and then their f-mean is evaluated, we get an upper bound of the arithmetic mean of the f-mean of the columns. In simple terms, the f-mean of arithmetic mean is lower bounded by the arithmetic mean of the f-mean. The proof is straightforward from Jensen’s inequality, and by noting that \( -\log \sum_i \exp(-t_i) \) is a concave function of \( t \). The last “\( \leq \)” leads to a proof of the upper bound in proposition 3.

**Remark 5.** The second complexity term on the RHS of eq. (11) is the f-mean of the quadratic term \( \frac{N}{2}(\theta - \hat{\theta})^T \mathcal{J}(\hat{\theta})(\theta - \hat{\theta}) \) w.r.t. the prior \( p(\theta) \), where \( f(t) = \exp(-t) \).

Based on the spectrum decomposition \( \mathcal{J}(\hat{\theta}) = \sum_{j=1}^D \lambda_j v_j v_j^T \) where the eigenvalues \( \lambda_j := \lambda_j(\hat{\theta}) \) and the eigenvectors \( v_j := v_j(\hat{\theta}) \) depend on the MLE \( \hat{\theta} \), we further write this term as

\[
\frac{N}{2}(\theta - \hat{\theta})^T \mathcal{J}(\hat{\theta})(\theta - \hat{\theta}) = \sum_{j=1}^D \frac{\lambda_j}{\text{tr}(\mathcal{J}(\hat{\theta}))} \cdot \frac{N}{2}\text{tr}(\mathcal{J}(\hat{\theta}))(\theta - \hat{\theta}, v_j)^2.
\]

By lemma 4, we have

\[
-\log \mathbb{E}_p \exp \left( -\frac{N}{2}(\theta - \hat{\theta})^T \mathcal{J}(\hat{\theta})(\theta - \hat{\theta}) \right) \geq -\sum_{j=1}^D \frac{\lambda_j}{\text{tr}(\mathcal{J}(\hat{\theta}))} \log \mathbb{E}_p \exp \left( -\frac{N}{2}\text{tr}(\mathcal{J}(\hat{\theta}))(\theta - \hat{\theta}, v_j)^2 \right).
\]
where the $f$-mean and the mean w.r.t. $\frac{N}{\text{tr}(\mathcal{J}(\hat{\theta}))}$ is swapped on the RHS.

Denote $\varphi_j = (\theta - \hat{\theta}, v_j)$. $\varphi = V^T(\theta - \hat{\theta})$ serves as a new coordinate system of $\mathcal{M}$, where $V$ is a $D \times D$ unitary matrix whose $j$'th column is $v_j$. The prior of $\varphi$ is given by $p(V\varphi + \hat{\theta})$. Then

$$
- \log E_p \exp \left( - \frac{N}{2} \text{tr}(\mathcal{J}(\hat{\theta}))(\theta - \hat{\theta}, v_j)^2 \right) = - \log E_p(\varphi_j) \exp \left( - \frac{N}{2} \text{tr}(\mathcal{J}(\hat{\theta}))\varphi_j^2 \right). \quad (13)
$$

Therefore, the model complexity has a lower bound, which is determined by the quantity $\frac{N}{2}\text{tr}(\mathcal{J}(\hat{\theta}))\varphi_j^2$ after evaluating the $f$-mean and some weighted mean, where $\varphi_j$ is an orthogonal transformation of the local coordinates $\theta$, based on the spectrum of $\mathcal{J}(\hat{\theta})$. Recall that the trace of the observed FIM $\mathcal{J}(\hat{\theta})$ means the overall amount of information a random observation contains w.r.t. the underlying model. Given the same sample size $N$, the larger $\text{tr}(\mathcal{J}(\hat{\theta}))$ is, the more complex the model is likely to be.

As $\hat{\theta}$ is the MLE, we have $\mathcal{J}(\hat{\theta}) = \mathcal{I}(\hat{\theta})$. Recall from eq. (7) that the FIM $\mathcal{I}(\hat{\theta})$ is a numerical average over all observed samples. We can have another lower bound of the model complexity based on lemma 4:

$$
- \log E_p \exp \left( - \frac{N}{2} (\theta - \hat{\theta})^T \mathcal{J}(\hat{\theta})(\theta - \hat{\theta}) \right) \geq - \frac{1}{N} N \sum_{i=1}^N \log E_p \exp \left( - \frac{N}{2} (\theta - \hat{\theta})^T \left( \frac{\partial h^L(z_i)}{\partial \theta} \right)^T C_i \frac{\partial h^L(z_i)}{\partial \theta} (\theta - \hat{\theta}) \right), \quad (14)
$$

where the $f$-mean and the numerical average of the samples are swapped on the RHS. Therefore the model complexity can be bounded by the average scale of the vector $\frac{\partial h^L(z_i)}{\partial \theta}(\theta - \hat{\theta})$, where $\theta \sim p(\theta)$. Note that $\frac{\partial h^L(z_i)}{\partial \theta}$ is the parameter-output Jacobian matrix, or a linear approximation of the neural network mapping $\theta \rightarrow h^L$. The complexity lower bound on the RHS of eq. (14) means how the local parameter change $\theta - \hat{\theta}$ w.r.t. the prior $p(\theta)$ affect the output. If the prior $p(\theta)$ is chosen so that the output is sensitive to the parameter variations, then the model is considered to have high complexity. As our model complexity is in the form of an $f$-mean, one can derive meaningful bounds and study its intuitive meanings.

### 7 The Razor based on Gaussian Prior

The simplest and most widely-used choice of the prior $p(\theta)$ is the Gaussian prior (see e.g. [30, 41] among many others). In eq. (12), we set

$$
\kappa(\theta) = \exp \left( -\theta^T \text{diag} \left( \frac{1}{\sigma} \right) \theta \right),
$$

where $\text{diag} (\cdot)$ means a diagonal matrix constructed with given entries, and $\sigma > 0$ (elementwisely).

Equivalently, $p_G(\theta) = \mathcal{G}(\theta | 0, \text{diag}(\sigma))$, meaning a Gaussian distribution with mean $0$ and covariance matrix $\text{diag}(\sigma)$. We further assume

(A4) $\mathcal{M}$ has a global coordinate chart and $\mathcal{M}$ is homeomorphic to $\mathbb{R}^D$.

(A5) Regardless of $D$, $\theta^T \text{diag} \left( \frac{1}{\sigma} \right) \theta < \infty$. 

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By assumption (A5), the MLE $\hat{\theta}$ has a non-zero probability under the Gaussian prior.

From eq. (12), we get a closed form expression (see appendix E for the derivations) of the razor

$$O_G := -\log p(X | \hat{\theta}) + \frac{\text{rank}(\hat{\mathcal{J}}(\hat{\theta}))}{2} \log N$$

$$+ \frac{1}{2} \sum_{i=1}^{\text{rank}(\hat{\mathcal{J}}(\hat{\theta}))} \log \left( \lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta})\text{diag}(\sigma)) + \frac{1}{N} \right) + O(1),$$

where $\lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta})\text{diag}(\sigma))$ denotes the $i$’th positive eigenvalue of $\hat{\mathcal{J}}(\hat{\theta})\text{diag}(\sigma)$. Notice that $\hat{\mathcal{J}}(\hat{\theta})\text{diag}(\sigma)$ and $\text{diag}(\sqrt{\sigma})\hat{\mathcal{J}}(\hat{\theta})\text{diag}(\sqrt{\sigma})$ share the same set of non-zero eigenvalues, and the latter is psd with $\text{rank}(\hat{\mathcal{J}}(\hat{\theta}))$ positive eigenvalues.

In our razor expressions, all terms that do not scale with the sample size $N$ or the number of parameters $D$ are discarded. The first two terms on the RHS are similar to BIC [63] up to scaling. To see the meaning of the third term on the RHS, we have

$$\sum_{i=1}^{\text{rank}(\hat{\mathcal{J}}(\hat{\theta}))} \log \left( \sigma_{\min}\lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta})) + \frac{1}{N} \right) \leq \sum_{i=1}^{\text{rank}(\hat{\mathcal{J}}(\hat{\theta}))} \log \left( \lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta})\text{diag}(\sigma)) + \frac{1}{N} \right) \leq \sum_{i=1}^{\text{rank}(\hat{\mathcal{J}}(\hat{\theta}))} \log \left( \sigma_{\max}\lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta})) + \frac{1}{N} \right),$$

where $\sigma_{\max}$ and $\sigma_{\min}$ denote the largest and smallest element of $\sigma$, respectively. Therefore the term can be bounded based on the spectrum of $\hat{\mathcal{J}}(\hat{\theta})$. If $D$ is large, we can also write the razor in terms of the spectrum density $\rho_T(\lambda)$, which is straightforward and omitted here for brevity.

The complexity terms (second and third terms on the RHS of eq. (15)) do not scale with $D$ but are bounded by the rank of the Hessian, or the observed FIM. In other words, the radical distribution associated with zero-eigenvalues of $\mathcal{J}(\theta)$ does not affect the model complexity. This is different from previous formulations of MDL [7, 59, 60] and BIC [63]. For example, the 2nd term on the RHS of eq. (2) increases linearly with $D$. Interestingly, if $\lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta})) < \frac{\sigma_{\max}}{\sigma_{\min}} (1 - \frac{1}{N})$, the third term on the RHS of eq. (15) becomes negative. In the extreme case when $\lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta}))$ tends to zero, $\frac{1}{2} \log \left( \sigma_{\max}\lambda_i^+ (\hat{\mathcal{J}}(\hat{\theta})) + \frac{1}{N} \right) \to -\frac{1}{2} \log N$, which cancels out the model complexity penalty in the term $\frac{\text{rank}(\hat{\mathcal{J}}(\hat{\theta}))}{2} \log N$. In other words, the corresponding parameter is added free (without increasing the model complexity). Informally, we call similar terms that are helpful in decreasing the complexity while contributing to model flexibility the negative complexity.

The Gaussian prior $p_G$ is helpful to give simple and intuitive expressions of $O_G$. However, the problem in choosing $p_G$ is two fold. First, it is not invariant. Under a reparametrization (e.g. normalization or centering techniques), the Gaussian prior in the new parameter system does not correspond to the original prior. Second, it double counts equivalent models. Because of the many singularities of the neuromanifold, a small dynamic in the parameter system may not change the prediction model. However, the Gaussian prior is defined in a real vector space and may not fit in this singular semi-Riemannian structure. Gaussian distributions are defined on Riemannian manifolds [62] which lead to potential extensions of the discussed prior $p_G(\theta)$. 

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Jeffreys' prior is specified by $p_J(\theta) \propto \sqrt{|I(\theta)|}$. It is non-informative in the sense that no neural network model $\theta_1$ is prioritized over any other model $\theta_2$. It is invariant to the choice of the coordinate system. Under a reparameterization $\theta \to \eta$,

$$\sqrt{|I(\eta)|}d\eta = \sqrt{\left(\frac{\partial \theta}{\partial \eta}^T I(\theta) \frac{\partial \theta}{\partial \eta}\right)} \cdot d\eta = \sqrt{|I(\theta)|} \cdot \left(\left|\frac{\partial \theta}{\partial \eta}\right| d\eta\right) = \sqrt{|I(\theta)|}d\theta,$$

showing that the Riemannian volume element is the same in different coordinate systems. Unfortunately, the Jeffreys' prior is not well defined on the lightlike neuromaniold $M$, where the metric $I(\theta)$ is degenerate and $\sqrt{|I(\theta)|}$ becomes zero. The stratifold structure of $M$, where $d(\theta)$ varying with $\theta \in M$, makes it difficult to properly define the base measure $d\theta$ and integrate functions as in eq. (12). From a mathematical standpoint, one has to integrate on the screen distribution $S(TM\mathcal{M})$, which has a Riemannian structure. We refer the reader to [29, 66] for other extensions of Jeffreys' prior.

In this paper, we take a simple approach by examining a submanifold of $\tilde{M}$ and parameterized by $\xi$, which has a Riemannian metric $\tilde{I}(\xi) > 0$ that is induced by the FIM $I(\theta) \succeq 0$. The dimensionality of $\tilde{M}$ is upper-bounded by the local dimensionality $d(\theta)$. Any infinitesimal dynamic on $\tilde{M}$ means such a change of neural network parameters that leads to a non-zero change of the global predictive model $z \to y$. Therefore, the following results are constrained to the choice of the submanifold $\tilde{M}$.

In eq. (12), let $s(\xi) = \sqrt{|\tilde{I}(\xi)|}$. We further assume

(A6) $0 < \int_{\tilde{M}} \sqrt{|\tilde{I}(\xi)|}d\xi < \infty$;

meaning that the Riemannian volume of $\tilde{M}$ is bounded. After straightforward derivations, we arrive at

$$O_J(\xi) = -\log p(X | \hat{\xi}) + \log \int_{\tilde{M}} \sqrt{|\tilde{I}(\xi)|}d\xi - \log \int_{\tilde{M}} \exp \left(-\frac{N}{2} (\xi - \hat{\xi})^T \bar{\mathcal{J}}(\xi)(\xi - \hat{\xi})\right) \sqrt{|\tilde{I}(\xi)|}d\xi. \tag{16}$$

Let us examine the meaning of $O_J(\xi)$. As $\tilde{I}(\xi)$ is the Riemannian metric of $\tilde{M}$ based on information geometry, $\sqrt{|\tilde{I}(\xi)|} \# d\xi$ is a Riemannian volume element (volume form). In the second term on the RHS of eq. (16), the integral $\int_{\tilde{M}} \sqrt{|\tilde{I}(\xi)|}d\xi$ is the information volume, or the total “number” of different DNN models [44] on $\tilde{M}$. In the last (third) term, because $\omega(\xi) := \exp \left(-\frac{N}{2} (\xi - \hat{\xi})^T \bar{\mathcal{J}}(\xi)(\xi - \hat{\xi})\right) \leq 1$, the integral on the LHS of

$$\int_{\tilde{M}} \exp \left(-\frac{N}{2} (\xi - \hat{\xi})^T \bar{\mathcal{J}}(\xi)(\xi - \hat{\xi})\right) \sqrt{|\tilde{I}(\xi)|}d\xi \leq \int_{\tilde{M}} \sqrt{|\tilde{I}(\xi)|}d\xi$$

means a “weighted volume” of $\tilde{M}$, where the weights $\omega(\xi)$ are determined by the observed FIM $\bar{\mathcal{J}}(\xi)$ and satisfy $0 < \omega(\xi) \leq 1$. Combining these two terms, the model complexity is the log-ratio between the unweighted volume and the weighted volume and is lower bounded by 0.

Assume the spectrum decomposition $\bar{\mathcal{J}}(\xi) = Q \text{diag} \left(\lambda_i(\bar{\mathcal{J}}(\xi))\right) Q^T$, where $Q$ has orthonormal

columns, and $\lambda_i(\mathcal{J}(\hat{\xi}))$ are the eigenvalues of $\mathcal{J}(\hat{\xi})$. Equation (16) becomes

$$
\mathcal{O}_J(\zeta) = -\log p(\mathbf{X} | \hat{\zeta}) + \log \int_{\tilde{\mathcal{M}}} \sqrt{|\mathcal{I}(\zeta)|} d\zeta
- \log \int_{\tilde{\mathcal{M}}} \exp \left( -\frac{N}{2} \sum_{i=1}^{\text{rank}(\mathcal{J}(\hat{\zeta}))} \lambda_i^+ (\mathcal{J}(\hat{\zeta})) (\zeta_i - \hat{\zeta}_i)^2 \right) \sqrt{|\mathcal{I}(\zeta)|} d\zeta,
$$

(17)

where $\zeta = Q^T \xi$ is an orthogonal transformation of $\xi$, and $\mathcal{O}_J$ is invariant to such transformations. If an eigenvalue of $\mathcal{J}(\hat{\xi})$ has an order of $o\left(\frac{1}{N}\right)$, the last two terms in eq. (17) cancel out in the corresponding direction, meaning no complexity is added. This is similar to how the positive and negative complexity terms cancel out in eq. (15) – small eigenvalues of $\mathcal{J}(\hat{\xi})$ are helpful to enhance the representation power of DNNs without increasing the model complexity. Only eigenvalues that are large enough contribute significantly to the model complexity.

In the rest of this section, we connect with previous formulations of MDL [7, 44]. If $\mathcal{J}(\hat{\xi})$ has full rank, we can further write

$$
\mathcal{O}_J(\hat{\mathcal{M}}) = -\log p(\mathbf{X} | \hat{\xi}) + \frac{\dim(\hat{\mathcal{M}})}{2} \log \frac{N}{2\pi} + \log \int_{\hat{\mathcal{M}}} \sqrt{|\mathcal{I}(\xi)|} d\xi
- \log \int_{\hat{\mathcal{M}}} G \left( \xi | \hat{\xi}, \frac{1}{N} J^{-1}(\hat{\xi}) \right) \frac{|\mathcal{I}(\xi)|^{1/2}}{|\mathcal{J}(\xi)|^{1/2}} d\xi.
$$

(18)

By assumption (A6), the RHS of eq. (16) is well defined, while the RHS of eq. (18) is only meaningful for a full rank $\mathcal{J}(\hat{\xi})$. If $\mathcal{J}(\hat{\xi})$ is not invertible, one can consider the limit case when the zero eigenvalues of $\mathcal{J}(\hat{\xi})$ are replaced by a small $\epsilon > 0$ and still enjoy the expression in eq. (18). One has to note that

$$
\int_{\hat{\mathcal{M}}} G \left( \xi | \hat{\xi}, \frac{1}{N} J^{-1}(\hat{\xi}) \right) \leq 1,
$$

as the internal is over $\hat{\mathcal{M}}$ which is a subset of $\mathbb{R}^{\dim(\hat{\mathcal{M}})}$. The last term on the RHS of eq. (18) resembles an expectation w.r.t. a Gaussian distribution centered at $\hat{\xi}$ on $\hat{\mathcal{M}}$, except the Gaussian density has been truncated by $\mathcal{M}$. One can therefore take the rough approximation based on the mean of the Gaussian:

$$
- \log \int_{\hat{\mathcal{M}}} G \left( \xi | \hat{\xi}, \frac{1}{N} J^{-1}(\hat{\xi}) \right) \frac{|\mathcal{I}(\xi)|^{1/2}}{|\mathcal{J}(\xi)|^{1/2}} d\xi \approx \frac{1}{2} \log \frac{|\mathcal{J}(\hat{\xi})|}{|\mathcal{I}(\hat{\xi})|}.
$$

(19)

Under this approximation, eq. (18) gives the MDL criterion discussed in [7, 44]. We therefore consider the spectrum of both matrices $\mathcal{I}(\xi)$ and $\mathcal{J}(\xi)$, noting that in the large sample limit $N \to \infty$, they become identical. Because of the finite $N$, the observed FIM $\mathcal{J}(\hat{\xi})$ is singular in potentially many directions. As a result, the log-ratio in eq. (19) serves as a negative complexity term and explains how singularities of $\mathcal{J}(\hat{\xi})$ correspond to the simplicity of DNNs.

Compared with $\mathcal{O}_G$, $\mathcal{O}_J$ is based on a more accurate geometric modeling. However, it is hard to be computed numerically. Despite that they have different expressions, their preference to model dimensions with small Fisher information (as in DNNs) is similar.

Hence, we can conclude that the intrinsic complexity of a DNN is affected by the singularity and spectral properties of the Fisher information matrix.
9 Related Work

The dynamics of supervised learning of a DNN describes a trajectory on the parameter space of the DNN geometrically modeled as a manifold when endowed with the FIM (e.g., ordinary/natural gradient descent learning the parameters of a MLP). Singular regions of the neuromanifold [71] correspond to non-identifiable parameters with rank-deficient FIM, and the learning trajectory typically exhibit chaotic patterns [4] with the singularities which translate into slowdown plateau phenomena when plotting the loss function value against time. By building an elementary singular DNN, [4] (and references therein) show that GD learning dynamics yields a Milnor-type attractor with both attractor/repulser subregions where the learning trajectory is attracted in the attractor region, then stay a long time there before escaping through the repulser region. The natural gradient is shown to be free of critical slowdowns. Furthermore, although DNNs have potentially many singular regions, it is shown that the interaction of elementary units cancels out the Milnor-type attractors. It was shown [49] that skip connections are helpful to reduce the effect of singularities. However, a full understanding of the learning dynamics [72] for generic DNN architectures with multiple output values or recurrent DNNs is yet to be investigated.

The MDL criterion has undergone several fundamental revisions, such as the original crude MDL [59] and refined MDL [8, 60]. We refer the reader to the book [22] for a comprehensive introduction to this area and [21] for a recent review. We should also mention that the relationship between MDL and generalization is not fully understood yet. See [21] for related remarks.

Our derivations based on a Taylor expansion of the log-likelihood are similar to [7]. This technique is also used for deriving natural gradient optimization for deep learning [4, 40, 51]. Recently MDL has been ported to deep learning [9] focusing on variational methods. MDL-related methods include weight sharing [18], binarization [27], model compression [12], etc.

In the deep learning community, there is a large body of literature on a theory of deep learning, for example, based on PAC-Bayes theory [47], statistical learning theory [73], algorithmic information theory [68], information geometry [39], geometry of the DNN mapping [56], or through defining an intrinsic dimensionality [38] that is much smaller than the network size. Our analysis depends on \( J(\hat{\theta}) \) and therefore is related to the flatness/sharpness of the local minima [13, 25].

Investigations are performed on the spectrum of the input-output Jacobian matrix \( \mathbf{J} \), the Hessian matrix w.r.t. the neural network weights [52], and the FIM [23, 30, 31, 50, 54].

10 Conclusion

We considered mathematical tools from singular semi-Riemannian geometry to study the locally varying intrinsic dimensionality of a deep learning model. These models fall in the category of non-identifiable parameterizations. We take a meaningful step to quantify geometric singularity through the notion of local dimensionality \( d(\theta) \) yielding a singular semi-Riemannian neuromanifold with varying metric signature. We show that \( d(\theta) \) grows at most linearly with the sample size \( N \). Recent findings show that the spectrum of the Fisher information matrix shifts towards 0 \( + \) with a large number of small eigenvalues. We show that these singular dimensions help to reduce the model complexity. As a result, we contribute a simple and general MDL for deep learning. It provides theoretical justifications on the description length of DNNs. DNNs benefit from a high-dimensional parameter space in that the singular dimensions impose a negative complexity to describe the data, which can be seen in our derivations based on Gaussian and Jeffreys’ priors. A more careful analysis of the FIM’s spectrum, e.g. through considering higher-order terms, could give more practical formulations of the proposed criterion. We leave empirical studies as potential future work.
Appendix A  Proof of $\hat{\mathcal{J}}(\hat{\theta}) = \mathcal{I}(\hat{\theta})$

Proof.

\[ p(y_i \mid z_i, \theta) = \exp \left( \text{OneHot}(y_i)^T h^L(z_i) - \log \sum_j \exp(h^L_j(z_i)) \right), \]

where $\text{OneHot}(y)$ is the binary vector with the same dimensionality as $h^L(z_i)$, with the $y$'th bit set to 1 and the rest bits set to 0. Therefore,

\[ \frac{\partial \log p(y_i \mid z_i, \theta)}{\partial \theta} = \left[ \frac{\partial h^L}{\partial \theta} \right]^T \left[ \text{OneHot}(y_i) - \text{SoftMax}(h^L(z_i)) \right]. \]

Therefore,

\[ \frac{\partial^2 \log p(y_i \mid z_i, \theta)}{\partial \theta \partial \theta^T} = \sum_j \left[ \text{OneHot}(y_i) - \text{SoftMax}(h^L(z_i)) \right]_j \frac{\partial^2 h^L_j}{\partial \theta \partial \theta^T} = \left[ \frac{\partial h^L}{\partial \theta} \right]^T C_i \cdot \frac{\partial h^L}{\partial \theta}, \quad (20) \]

where

\[ C_i = \frac{\partial \text{SoftMax}(h^L(z_i))}{\partial h^L(z_i)} = \text{diag}(o_i) - o_i o_i^T, \quad o_i = \text{SoftMax}(h^L(z_i)). \]

By (A1), at the MLE $\hat{\theta}$,

\[ \forall i, \quad \text{SoftMax}(h^L(z_i)) = \text{OneHot}(y_i). \]

Therefore

\[ \forall i, \quad - \frac{\partial^2 \log p(y_i \mid z_i, \theta)}{\partial \theta \partial \theta^T} = \left[ \frac{\partial h^L}{\partial \theta} \right]^T C_i \cdot \frac{\partial h^L}{\partial \theta}. \]

Taking the sample average on both sides, we get

\[ \hat{\mathcal{J}}(\hat{\theta}) = \mathcal{I}(\hat{\theta}). \]

\[ \square \]

Appendix B  Proof of Lemma 1

Proof. If $(\theta, \sum_j \alpha_j \partial \theta_j) \in \text{Rad}(\mathcal{M})$, Then

\[ \left\langle \sum_j \alpha_j \partial \theta_j, \sum_j \alpha_j \partial \theta_j \right\rangle_{\mathcal{I}(\theta)} = 0. \]

In matrix form, it is simply $\alpha^T \mathcal{I}(\theta) \alpha = 0$. We have the analytical expression

\[ \mathcal{I}(\theta) = \mathbb{E}_p \left[ \left( \frac{\partial h^L(z)}{\partial \theta} \right)^T C(z) \frac{\partial h^L(z)}{\partial \theta} \right]. \]

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Therefore

\[ E_p \left[ \left( \frac{\partial h^L(z)}{\partial \theta} \alpha \right)^\top C(z) \frac{\partial h^L(z)}{\partial \theta} \alpha \right] = 0. \]

By noting that \( C(z) \succeq 0 \) is psd, we have almost surely that

\[ \left( \frac{\partial h^L(z)}{\partial \theta} \alpha \right)^\top C(z) \frac{\partial h^L(z)}{\partial \theta} \alpha = 0. \]

Any eigenvector of \( C(z) \) associated with the zero eigenvalues must be a multiple of \( 1 \). Indeed,

\[ v^\top C(z) v = v^\top (\text{diag}(o(z)) - o(z)o(z)^\top) v = \sum_j o_j(z)(v_j - \sum_j o_j(z)v_j)^2 = 0 \iff v \propto 1, \]

where \( o_j(z) > 0 \) is the \( j \)'th element of \( o(z) \). Hence, almost surely

\[ \frac{\partial h^L(z)}{\partial \theta} \alpha = \lambda(z)1. \]

\[ \square \]

Remark. \( \alpha \) is associated with a tangent vector in \( \text{Rad}(\mathcal{T}, \mathcal{M}) \), meaning a dynamic along the lightlike dimensions. The Jacobian \( \frac{\partial h^L(z)}{\partial \theta} \) is the local linear approximation of the mapping \( \theta \rightarrow h^L(z) \). By lemma 1, with probability 1 such a dynamic leads to uniform increments in the output units, meaning \( h^L(z) \rightarrow h^L(z) + \lambda(z)1, \forall i \), and therefore the output distribution \( \text{SoftMax}\left(h^L(z)\right) \) is not affected. In summary, we have verified that the radical distribution does not affect the neural network mapping.

Appendix C  Proof of Proposition 2

Proof.

\[ \tilde{d}(\theta) = \text{rank}\left( \mathcal{I}(\theta) \right) = \text{rank}\left( \sum_{i=1}^N \left( \frac{\partial h^L(z_i)}{\partial \theta} \right)^\top \mathcal{C}_i \frac{\partial h^L(z_i)}{\partial \theta} \right) \leq \sum_{i=1}^N \text{rank}\left( \left( \frac{\partial h^L(z_i)}{\partial \theta} \right)^\top \mathcal{C}_i \frac{\partial h^L(z_i)}{\partial \theta} \right) \leq (m - 1)N. \]

Note the matrix \( \frac{\partial h^L(z_i)}{\partial \theta} \) has size \( m \times D \), and \( \mathcal{C}_i \) has size \( m \times m \) and rank \( (m - 1) \). We also have \( \tilde{d}(\theta) = \text{rank}\left( \mathcal{I}(\theta) \right) \leq D = \text{dim}(\theta) \). Therefore

\[ \tilde{d}(\theta) \leq \min(D, (m - 1)N). \]

\[ \square \]

The metric signature of \( \mathcal{M} \)

\[ (d(\theta), 0, D - d(\theta)) \]

is straightforward from the fact that \( \mathcal{I}(\theta) \) is positive semi-definite (there is no negative eigenvalues), and the local dimensionality \( d(\theta) \), by definition, is rank \( (\mathcal{I}(\theta)) \) (the number of non-zero eigenvalues).
We also show that \( \text{rank}(\hat{\mathcal{J}}(\theta)) \neq \hat{d}(\theta) \). Recall that \( \hat{d}(\theta) = \text{rank}(\hat{\mathcal{I}}(\theta)) \), and

\[
\text{rank}(\mathcal{J}(\theta)) = \text{rank}\left( \frac{\partial^2 \ell}{\partial \theta \theta^\top} \right) = \text{rank}\left( \sum_i \frac{\partial^2 \ell_i}{\partial \theta \theta^\top} \right),
\]

where \( \ell \) is the log-likelihood, and \( \ell_i = \log p(y_i | z_i, \theta) \). We write the analytical form of the elementwise Hessian

\[
\frac{\partial^2 \ell_i}{\partial \theta \partial \theta^\top} = \sum_{j=1}^m \frac{\partial h^L_j(z_i)}{\partial \theta \partial \theta^\top} \left( \text{OneHot}_j(y) - \text{SoftMax}_j(h^L) \right) - I(\theta),
\]

where \( \text{OneHot}(\cdot) \) denote the one-hot vector associated with the given target label \( y \). Therefore

\[
\alpha^\top \frac{\partial^2 \ell_i}{\partial \theta \partial \theta^\top} \alpha = \sum_{j=1}^m \alpha^\top \left( \frac{\partial h^L_j(z_i)}{\partial \theta \partial \theta^\top} \right) \left( \text{OneHot}_j(y) - \text{SoftMax}_j(h^L) \right) - \alpha^\top \mathcal{I}(\theta) \alpha.
\]

Because of the first term on the RHS, the kernels of the two matrices \( \mathcal{J}(\theta) \) and \( \hat{\mathcal{I}}(\theta) \) are different, and thus their ranks are also different.

### Appendix D Proof of Proposition 3

**Proof.** As \( \hat{\theta} \) is the MLE, we have \( \mathcal{J}(\hat{\theta}) \succeq 0 \), and \( \forall \theta \in \mathcal{M}, \)

\[
-\frac{N}{2} (\theta - \hat{\theta})^\top \mathcal{J}(\theta)(\theta - \hat{\theta}) \leq 0.
\]

Hence,

\[
\mathbb{E}_p \exp \left( -\frac{N}{2} (\theta - \hat{\theta})^\top \mathcal{J}(\theta)(\theta - \hat{\theta}) \right) \leq 1.
\]

Hence,

\[
-\log \mathbb{E}_p \exp \left( -\frac{N}{2} (\theta - \hat{\theta})^\top \mathcal{J}(\theta)(\theta - \hat{\theta}) \right) \geq 0.
\]

This proves the first “\( \leq \)”.

As \( -\log(x) \) is convex, by Jensen’s inequality, we get

\[
-\log \mathbb{E}_p \exp \left( -\frac{N}{2} (\theta - \hat{\theta})^\top \mathcal{J}(\theta)(\theta - \hat{\theta}) \right) \leq \mathbb{E}_p \left( -\log \exp \left( -\frac{N}{2} (\theta - \hat{\theta})^\top \mathcal{J}(\theta)(\theta - \hat{\theta}) \right) \right)
\]

\[
= \mathbb{E}_p \left( \frac{N}{2} (\theta - \hat{\theta})^\top \mathcal{J}(\theta)(\theta - \hat{\theta}) \right)
\]

\[
= \frac{N}{2} \text{tr} \left( \mathcal{J}(\theta)(\theta - \hat{\theta})(\theta - \hat{\theta})^\top \right)
\]

\[
= \frac{N}{2} \text{tr} \left( \mathcal{J}(\theta) \left( (\mu(\theta) - \hat{\theta})(\mu(\theta) - \hat{\theta})^\top + \text{cov}(\theta) \right) \right).
\]

This proves the second “\( \leq \)”.

\[\square\]
Appendix E Derivations of $\mathcal{O}_G$

We recall the general formulation in eq. (12):

$$
\mathcal{O} := -\log p(X | \hat{\theta}) + \log \int_{\mathcal{M}} \kappa(\theta) d\theta - \log \int_{\mathcal{M}} \kappa(\theta) \exp \left( -\frac{N}{2} (\theta - \hat{\theta})^T \hat{\Sigma}(\hat{\theta})(\theta - \hat{\theta}) \right) d\theta.
$$

If $\kappa(\theta) = \exp \left( -\frac{1}{2} \theta^T \text{diag} \left( \frac{1}{\sigma} \right) \theta \right)$, then the second term on the RHS is

$$
\log \int_{\mathcal{M}} \kappa(\theta) d\theta = \log \int_{\mathcal{M}} \exp \left( -\frac{1}{2} \theta^T \text{diag} \left( \frac{1}{\sigma} \right) \theta \right) d\theta
= \frac{D}{2} \log 2\pi + \frac{1}{2} \log |\text{diag} (\sigma)|
+ \log \int_{\mathcal{M}} \exp \left( -\frac{D}{2} \log 2\pi - \frac{1}{2} \theta^T \text{diag} \left( \frac{1}{\sigma} \right) \theta \right) d\theta
= \frac{D}{2} \log 2\pi + \frac{1}{2} \log |\text{diag} (\sigma)|.
$$

The third (last) term on the RHS is

$$
-\log \int_{\mathcal{M}} \kappa(\theta) \exp \left( -\frac{N}{2} (\theta - \hat{\theta})^T \hat{\Sigma}(\hat{\theta})(\theta - \hat{\theta}) \right) d\theta
= -\log \int_{\mathcal{M}} \exp \left( -\frac{1}{2} \theta^T \text{diag} \left( \frac{1}{\sigma} \right) \theta - \frac{N}{2} (\theta - \hat{\theta})^T \hat{\Sigma}(\hat{\theta})(\theta - \hat{\theta}) \right) d\theta
= -\log \int_{\mathcal{M}} \exp \left( -\frac{1}{2} \theta^T A \theta + b^T \theta + c \right) d\theta,
$$

where

$$
A = N \hat{\Sigma}(\hat{\theta}) + \text{diag} \left( \frac{1}{\sigma} \right) \succ 0, \quad b = N \hat{\Sigma}(\hat{\theta}) \hat{\theta}, \quad c = -\frac{N}{2} \hat{\theta}^T \hat{\Sigma}(\hat{\theta}) \hat{\theta}.
$$

Then,

$$
-\log \int_{\mathcal{M}} \kappa(\theta) \exp \left( -\frac{N}{2} (\theta - \hat{\theta})^T \hat{\Sigma}(\hat{\theta})(\theta - \hat{\theta}) \right) d\theta
= -\log \int_{\mathcal{M}} \exp \left( -\frac{1}{2} (\theta - \hat{\theta})^T A (\theta - \hat{\theta}) + c + \frac{1}{2} \hat{\theta}^T A \hat{\theta} \right) d\theta
= -\frac{D}{2} \log 2\pi + \frac{1}{2} \log |A| - c - \frac{1}{2} \hat{\theta}^T A \hat{\theta}
-\log \int_{\mathcal{M}} \exp \left( -\frac{D}{2} \log 2\pi + \frac{1}{2} \log |A| - \frac{1}{2} (\theta - \hat{\theta})^T A (\theta - \hat{\theta}) \right) d\theta
= -\frac{D}{2} \log 2\pi + \frac{1}{2} \log |A| - c - \frac{1}{2} \hat{\theta}^T A \hat{\theta},
$$

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where \( \mathbf{A} \hat{\theta} = b \). To sum up,

\[
O_G = -\log p(\mathbf{X} | \hat{\theta}) + \frac{D}{2} \log 2\pi + \frac{1}{2} \log |\text{diag}(\sigma)| + \frac{D}{2} \log 2\pi + \frac{1}{2} \text{log} |\mathbf{A}| - c - \frac{1}{2} \hat{\theta}^T \mathbf{A} \hat{\theta}
\]

\[
= -\log p(\mathbf{X} | \hat{\theta}) + \frac{1}{2} \text{log} |\text{diag}(\sigma)| + \frac{1}{2} \text{log} |\mathbf{A}| - c - \frac{1}{2} \hat{\theta}^T \mathbf{A} \hat{\theta},
\]

where \( c \) is a constant. By assumption (A5), the RHS is

\[
\text{rank} \mathbf{O} = \text{rank} \mathbf{G} = \text{rank} \bar{\mathbf{G}} = \text{rank} \mathbf{L}(\hat{\theta}) \mathbf{L}(\hat{\theta})^\top.
\]

By the Weinstein–Aronszajn identity, the identity matrix of shape \( \mathbf{O} \) and has a smaller order as compared to other terms. Indeed,

\[
\text{rank} \mathbf{O} = \text{rank} \mathbf{G} = \text{rank} \bar{\mathbf{G}} = \text{rank} \mathbf{L}(\hat{\theta}) \mathbf{L}(\hat{\theta})^\top.
\]

This term is therefore dropped. We get

\[
O_G = -\log p(\mathbf{X} | \hat{\theta}) + \frac{1}{2} \text{log} |\text{diag}(\sigma)| + \frac{1}{2} \text{log} |\mathbf{A}| - c - \frac{1}{2} \hat{\theta}^T \mathbf{A} \hat{\theta}.
\]

The last term does not scale with \( N \) and has a smaller order as compared to other terms. Indeed, as \( N \to \infty \), \( \left( \mathbf{N} \mathbf{J}(\hat{\theta}) \mathbf{J}(\hat{\theta})^\top + \frac{1}{N} \text{diag} \left( \frac{1}{\sigma} \right) \right)^{-1} \to \mathbf{N} \mathbf{J}(\hat{\theta})^+ \), the Moore–Penrose inverse of \( \mathbf{N} \mathbf{J}(\hat{\theta}) \). Hence,

\[
\frac{1}{2} \hat{\theta}^T \mathbf{J}(\hat{\theta}) \left( \text{diag}(\sigma) \mathbf{J}(\hat{\theta}) + \frac{1}{N} \mathbf{I} \right)^{-1} \mathbf{J}(\hat{\theta})^+ \text{diag} \left( \frac{1}{\sigma} \right) \hat{\theta} \leq \frac{1}{2} \hat{\theta}^T \text{diag} \left( \frac{1}{\sigma} \right) \hat{\theta}.
\]

By assumption (A5), the RHS is \( O(1) \). This term is therefore dropped. We get

\[
O_G = -\log p(\mathbf{X} | \hat{\theta}) + \frac{1}{2} \text{log} |\text{diag}(\sigma)| + \frac{1}{2} \text{log} |\mathbf{A}| - c - \frac{1}{2} \hat{\theta}^T \mathbf{A} \hat{\theta}.
\]

Note that rank \( \mathbf{J}(\hat{\theta}) \leq D \), and the matrix \( \mathbf{J}(\hat{\theta})\text{diag}(\sigma) \) has the same rank as \( \mathbf{J}(\hat{\theta}) \). We can write \( \mathbf{J}(\hat{\theta}) = \mathbf{L}(\hat{\theta}) \mathbf{L}(\hat{\theta})^\top \), where \( \mathbf{L}(\hat{\theta}) \) has shape \( D \times \text{rank} \left( \mathbf{J}(\hat{\theta}) \right) \). We abuse \( \mathbf{I} \) to denote both the identity matrix of shape \( D \times D \) and the identity matrix of shape \( \text{rank} \left( \mathbf{J}(\hat{\theta}) \right) \times \text{rank} \left( \mathbf{J}(\hat{\theta}) \right) \).

By the Weinstein–Aronszajn identity,

\[
O_G = -\log p(\mathbf{X} | \hat{\theta}) + \frac{1}{2} \text{log} \left| \mathbf{N} \mathbf{L}(\hat{\theta}) \mathbf{L}(\hat{\theta})^\top \text{diag}(\sigma) + \mathbf{I} \right| + O(1)
\]

\[
= -\log p(\mathbf{X} | \hat{\theta}) + \frac{1}{2} \text{log} \left| \mathbf{N} \mathbf{L}(\hat{\theta})^\top \text{diag}(\sigma) \mathbf{L}(\hat{\theta}) + \mathbf{I} \right| + O(1)
\]

\[
= -\log p(\mathbf{X} | \hat{\theta}) + \frac{\text{rank} \left( \mathbf{J}(\hat{\theta}) \right)}{2} \text{log} N + \frac{1}{2} \text{log} \left| \mathbf{L}(\hat{\theta})^\top \text{diag}(\sigma) \mathbf{L}(\hat{\theta}) + \frac{1}{N} \mathbf{I} \right| + O(1).
\]
Note \( L(\hat{\theta})^T \text{diag}(\sigma) L(\hat{\theta}) \) have the same set of non-zero eigenvalues as \( L(\hat{\theta}) L(\hat{\theta})^T \text{diag}(\sigma) = \tilde{\sigma}(\hat{\theta}) \text{diag}(\sigma) \), which we denote as \( \lambda^+\left(\tilde{\sigma}(\hat{\theta}) \text{diag}(\sigma)\right) \). Then,

\[
O_G = - \log p(X | \hat{\theta}) + \frac{\text{rank}(\tilde{\sigma}(\hat{\theta}))}{2} \log N \\
+ \frac{1}{2} \sum_{i=1}^{\text{rank}(\tilde{\sigma}(\hat{\theta}))} \log \left( \lambda^+_i \left(\tilde{\sigma}(\hat{\theta}) \text{diag}(\sigma)\right) + \frac{1}{N} \right) + O(1).
\]

Denote the largest/smallest element of \( \sigma \) as \( \sigma_{\max} \) and \( \sigma_{\min} \), respectively. Then,

\[
L(\hat{\theta})^T \text{diag}(\sigma) L(\hat{\theta}) \preceq \sigma_{\max} L(\hat{\theta})^T L(\hat{\theta}).
\]

Hence,

\[
\frac{1}{2} \log \left| L(\hat{\theta})^T \text{diag}(\sigma) L(\hat{\theta}) + \frac{1}{N} I \right| \leq \frac{1}{2} \log \left| \sigma_{\max} L(\hat{\theta})^T L(\hat{\theta}) + \frac{1}{N} I \right|
\]

\[
= \frac{1}{2} \sum_{i=1}^{\text{rank}(\tilde{\sigma}(\hat{\theta}))} \log \left( \sigma_{\max} \lambda^+_i \left(\tilde{\sigma}(\hat{\theta})\right) + \frac{1}{N} \right).
\]

Similarly,

\[
\frac{1}{2} \log \left| L(\hat{\theta})^T \text{diag}(\sigma) L(\hat{\theta}) + \frac{1}{N} I \right| \geq \frac{1}{2} \sum_{i=1}^{\text{rank}(\tilde{\sigma}(\hat{\theta}))} \log \left( \sigma_{\min} \lambda^+_i \left(\tilde{\sigma}(\hat{\theta})\right) + \frac{1}{N} \right).
\]

If \( \sigma = \sigma 1 \), then \( \sigma_{\max} = \sigma_{\min} = \sigma \). Both “\( \leq \)” and “\( \geq \)” in the above inequalities become tight.

**Appendix F  Probability Measures on \( \mathcal{M} \)**

Probability measures are not defined on the lightlike \( \mathcal{M} \), because along the lightlike geodesics, the distance is zero. To compute the integral of a given function \( f(\theta) \) on \( \mathcal{M} \) one has to first choose a proper Riemannian submanifold \( \mathcal{M}^s \subset \mathcal{M} \) specified by an embedding \( \theta(\theta^s) \), whose metric is not singular. Then, the integral on \( \mathcal{M}^s \) can be defined as \( \int_{\mathcal{M}^s} f(\theta(\theta^s)) d\theta^s \), where \( \mathcal{M}^s \) is the sub-manifold associated with the frame \( \theta^s = (\theta^1, \ldots, \theta^d) \), so that \( T \mathcal{M}^s = S(\mathcal{T} \mathcal{M}) \), and the induced Riemannian volume element as

\[
d\theta^s = \sqrt{|I(\theta^s)|} \ d\theta^1 \wedge d\theta^2 \wedge \cdots \wedge d\theta^d
\]

\[
= \sqrt{|I(\theta^s)|} \ dE_{\theta^s}, \tag{21}
\]

where \( dE_{\theta} \) is the Euclidean volume element. We artificially shift \( \theta \) to be positive definite and define the volume element as

\[
d\theta := \sqrt{|I(\theta)| + \varepsilon_1 I_0} \ d\theta^1 \wedge d\theta^2 \wedge \cdots \wedge d\theta^D
\]

\[
= \sqrt{|I(\theta)| + \varepsilon_1 I} \ dE_{\theta}, \tag{22}
\]

where \( \varepsilon_1 > 0 \) is a very small value as compared to the scale of \( I(\theta) \) given by \( \frac{1}{N} \text{tr}(I(\theta)) \), i.e. the average of its eigenvalues. Notice this element will vary with \( \theta \): different coordinate systems will
yield different volumes. Therefore it depends on how \( \theta \) can be uniquely specified. This is roughly guaranteed by our A1: the \( \theta \)-coordinates correspond to the input coordinates (weights and biases) up to an orthogonal transformation. Despite that eq. (22) is a loose mathematical definition, it makes intuitive sense and is convenient for making derivations. Then, we can integrate functions

\[
\int_{\mathcal{M}} f(\theta) d\theta = \int f(\theta) \sqrt{|\mathcal{I}(\theta)| + \varepsilon_1 I} \, d\mathbf{e}_\theta,
\]

where the RHS is an integration over \( \mathbb{R}^D \), assuming \( \theta \) is real-valued.

Using this tool, we first consider Jeffreys’ non-informative prior on a sub-manifold \( \mathcal{M}^* \), given by

\[
p_j(\theta^*) = \frac{\sqrt{|\mathcal{I}(\theta^*)|}}{\int_{\mathcal{M}^*} \sqrt{|\mathcal{I}(\theta^*)|} \, d\mathbf{e}_\theta^*}.
\]

It is easy to check \( \int_{\mathcal{M}^*} p(\theta^*) \, d\mathbf{e}_\theta^* = 1 \). This prior may lead to similar results as [7, 60], i.e. a “razor” of the model \( \mathcal{M}^* \). However, we will instead use a Gaussian-like prior, because Jeffreys’ prior is not well defined on \( \mathcal{M} \). Moreover, the integral \( \int_{\mathcal{M}^*} \sqrt{|\mathcal{I}(\theta^*)|} \, d\mathbf{e}_\theta^* \) is likely to diverge based on our revised volume element in eq. (22). If the parameter space is real-valued, one can easily check that, the volume based on eq. (22) along the lightlike dimensions will diverge. The zero-centered Gaussian prior corresponds to a better \( \text{code} \), because it is commonly acknowledged that one can achieve the same training error and generalization without using large weights. For example, regularizing the norm of the weights is widely used in deep learning. By using such an informative prior, one can have the same training error in the first term in eq. (2), while having a smaller “complexity” in the rest of the terms, because we only encode such models with constrained weights. Given the DNN, we define an informative prior on the lightlike neuromanifold

\[
p(\theta) = \frac{1}{V} \exp \left( -\frac{1}{2\varepsilon_2^2} \| \theta \|^2 \right) \sqrt{|\mathcal{I}(\theta)| + \varepsilon_1 I},
\]

where \( \varepsilon_2 > 0 \) is a scale parameter of \( \theta \), and \( V \) is a normalizing constant to ensure \( \int p(\theta) d\mathbf{e}_\theta = 1 \).

Here, the base measure is the Euclidean volume element \( d\mathbf{e}_\theta \), as \( \sqrt{|\mathcal{I}(\theta)| + \varepsilon_1 I} \) already appeared in \( p(\theta) \). Keep in mind, again, that this \( p(\theta) \) is defined in a special coordinate system, and is not invariant to re-parametrization. By A1, this distribution is also isotropic in the input coordinate system, which agrees with initialization techniques\(^7\).

This bi-parametric prior connects Jeffreys’ prior (that is widely used in MDL) and a Gaussian prior (that is widely used in deep learning). If \( \varepsilon_2 \to \infty \), \( \varepsilon_1 \to 0 \), it coincides with Jeffreys’ prior (if it is well defined and \( \mathcal{I}(\theta) \) has full rank); if \( \varepsilon_1 \) is large, the metric \( (\mathcal{I}(\theta) + \varepsilon_1 I) \) becomes spherical, and eq. (25) becomes a Gaussian prior. We refer the reader to [29, 66] for other extensions of Jeffreys’ prior.

The normalizing constant of eq. (25) is an information volume measure of \( \mathcal{M} \), given by

\[
V := \int_{\mathcal{M}} \exp \left( -\frac{1}{2\varepsilon_2^2} \| \theta \|^2 \right) \, d\theta.
\]

Unlike Jeffreys’ prior whose information volume (the 3rd term on the RHS of eq. (2)) can be unbounded, this volume is better bounded by

**Theorem 5.**

\[
(\sqrt{2\pi\varepsilon_1\varepsilon_2})^D \leq V \leq (\sqrt{2\pi(\varepsilon_1 + \lambda_m)\varepsilon_2})^D,
\]

where \( \lambda_m \) is the largest eigenvalue of the FIM \( \mathcal{I}(\theta) \).

\(^7\)Different layers, or weights and biases, may use different variance in their initialization. This minor issue can be solved by a simple re-scaling re-parameterization.
Notice $\lambda_m$ may not exist, as the integration is taken over $\theta \in \mathcal{M}$. Intuitively, $V$ is a weighted volume w.r.t. a Gaussian-like prior distribution on $\mathcal{M}$, while the 3rd term on the RHS of eq. (2) is an unweighted volume. The larger the radius $\varepsilon_2$, the more “number” or possibilities of DNNs are included; the larger the parameter $\varepsilon_1$, the larger the local volume element in eq. (22) is measured, and therefore the total volume is measured larger. $\log V$ is an $O(D)$ terms, meaning the volume grows with the number of dimensions.

F.1 Proof of Theorem 5

By definition,

$$V = \int_\mathcal{M} \exp \left( -\frac{1}{2\varepsilon_2^2} \|\theta\|^2 \right) d\theta = \int \exp \left( -\frac{1}{2\varepsilon_2^2} \|\theta\|^2 \right) \sqrt{|\mathcal{I}(\theta) + \varepsilon_1 I|} d\theta.$$

By (A1), $\theta$ is an orthogonal transformation of the neural network weights and biases, and therefore $\theta \in \mathbb{R}^D$. We have

$$\sqrt{|\mathcal{I}(\theta) + \varepsilon_1 I|} \geq \sqrt{\varepsilon_1 I} = \varepsilon_1^\frac{D}{2}.$$

Hence

$$V \geq \int \exp \left( -\frac{1}{2\varepsilon_2^2} \|\theta\|^2 \right) \varepsilon_1^\frac{D}{2} d\theta \varepsilon_1^{\frac{D}{2}} = (2\pi)^\frac{D}{2} \varepsilon_2^D \varepsilon_1^\frac{D}{2} = (\sqrt{2\pi\varepsilon_1 \varepsilon_2})^D.$$

For the upper bound, we prove a stronger result as follows.

$$\sqrt{|\mathcal{I}(\theta) + \varepsilon_1 I|} = \left( \prod_{i=1}^{D} (\lambda_i + \varepsilon_1)^\frac{1}{2} \right) \leq \left( \frac{1}{D} \text{tr}(\mathcal{I}(\theta)) + \varepsilon_1 \right)^\frac{D}{2}.$$

Therefore

$$V \leq \left( \sqrt{2\pi\varepsilon_2} \right)^D \left( \frac{1}{D} \text{tr}(\mathcal{I}(\theta)) + \varepsilon_1 \right)^\frac{D}{2}.$$

If one applies $\frac{1}{D} \text{tr}(\mathcal{I}(\theta)) \leq \lambda_m$ to the RHS, the upper bound is further relaxed as

$$V \leq \left( \sqrt{2\pi\varepsilon_2} \right)^D (\lambda_m + \varepsilon_1)^\frac{D}{2} = \left( \sqrt{2\pi(\varepsilon_1 + \lambda_m)\varepsilon_2} \right)^D.$$

Appendix G An Alternative Derivation of the Razor

In this section, we provide an alternative derivation of the propose razor $O$ based on a different prior. The main observations on the negative complexity is consistent with the cases of Gaussian and Jeffreys’ priors.

We plug in the expression of $p(\theta)$ in eq. (25) and get

$$- \log p(X) \approx - \log p(X | \theta) + \log V$$

$$- \log \int_\mathcal{M} \left( -\frac{\|\theta\|^2}{2\varepsilon_2^2} - \frac{N}{2}(\theta - \hat{\theta})^T \mathcal{I}(\theta) (\theta - \hat{\theta}) \right) d\theta.$$
In the last term on the RHS, inside the parentheses is a quadratic function w.r.t. \( \theta \). However the integration is w.r.t. to the non-Euclidean volume element \( d\theta \) and therefore does not have closed form. We need to assume

\[ (A3) \quad N \text{ is large enough so that } |I(\theta) + \varepsilon_1 I| \approx |I(\hat{\theta}) + \varepsilon_1 I|. \]

This means the quadratic function will be sharp enough to make the volume element \( d\theta \) to be roughly constant. Along the lightlike dimensions (zero eigenvalues of \( I(\theta) \)) this is trivial.

Plug eq. (25) into eq. (10), the following three terms

\[ \frac{1}{V}, \quad \sqrt{|I(\theta) + \varepsilon_1 I|} \approx \sqrt{|I(\hat{\theta}) + \varepsilon_1 I|}, \quad \exp \left( \log p(X | \hat{\theta}) \right) = p(X | \hat{\theta}) \]

can all be taken out of the integration as constant scalers, as they do not depend on \( \theta \). The main difficulty is to perform the integration

\[ \int \exp \left( -\frac{\| \theta \|^2}{2\varepsilon_2^2} - \frac{N}{2}(\theta - \hat{\theta})^T \mathcal{J}(\hat{\theta})(\theta - \hat{\theta}) \right) d\theta \]

where

\[ \mathcal{A} = N\mathcal{J}(\hat{\theta}) + \frac{1}{\varepsilon_2^2} I, \quad \mathcal{B} = N\mathcal{J}(\hat{\theta})\hat{\theta}, \quad c = -\frac{1}{2} \theta^T N\mathcal{J}(\hat{\theta}) \hat{\theta}. \]

The rest of the derivations are straightforward. Note \( R = -c - \frac{1}{2} \mathcal{B}^T \mathcal{A}^{-1} \mathcal{B} \).

After derivations and simplifications, we get

\[ -\log p(X) \approx -\log p(X | \hat{\theta}) + \frac{D}{2} \log \frac{N}{2\pi} + \log V \]

\[ + \frac{1}{2} \log \left| \mathcal{J}(\hat{\theta}) + \frac{1}{N\varepsilon_2^2} I \right| - \frac{1}{2} \log |I(\hat{\theta}) + \varepsilon_1 I| + R. \]

The remainder term is given by

\[ R = \frac{1}{2} \hat{\theta}^T \left[ N\mathcal{J}(\hat{\theta}) - N\mathcal{J}(\hat{\theta}) \left( N\mathcal{J}(\hat{\theta}) + \frac{1}{\varepsilon_2^2} I \right)^{-1} N\mathcal{J}(\hat{\theta}) \right] \hat{\theta}. \]

We need to analyze the order of this \( R \) term. Assume the largest eigenvalue of \( \mathcal{J}(\hat{\theta}) \) is \( \lambda_m \), then

\[ |R| \leq \frac{N\lambda_m}{\varepsilon_2^2 N\lambda_m + 1} \| \hat{\theta} \|^2. \]

We assume
Figure 2: A: a model far from the truth (underlying distribution of observed data); B: close to the truth but sensitive to parameter; C (deep learning): close to the truth with many good local optima.

\[(A7)\] The ratio between the scale of each dimension of the MLE \(\hat{\theta}\) to \(\varepsilon_2\), i.e. \(\frac{\hat{\theta}_i}{\varepsilon_2}\) \(i = 1, \cdots, D\) is in the order \(O(1)\).

Intuitively, the scale parameter \(\varepsilon_2\) in our prior \(p(\theta)\) in eq. (25) is chosen to “cover” the good models. Therefore, the order of \(R\) is \(O(D)\). As \(N\) turns large, \(R\) will be dominated by the 2nd \(O(D \log N)\) term. We will therefore discard \(R\) for simplicity. It could be useful for a more delicate analysis. In conclusion, we arrive at the following expression

\[
\mathcal{O} := -\log p(X | \hat{\theta}) + \frac{D}{2} \log \frac{N}{2\pi} + \log V + \frac{1}{2} \log \frac{3(\hat{\theta}) + \frac{1}{N \varepsilon_2^2} I}{I(\hat{\theta}) + \varepsilon_1 I}. \tag{31}
\]

Notice the similarity with eq. (2), where the first two terms on the RHS are exactly the same. The 3rd term is an \(O(D)\) term, similar to the 3rd term in eq. (2). It is bounded according to theorem 5, while the 3rd term in eq. (2) could be unbounded. Our last term is in a similar form to the last term in eq. (2), except it is well defined on lightlike manifold. If we let \(\varepsilon_2 \to \infty, \varepsilon_1 \to 0\), we get exactly eq. (2) and in this case \(\mathcal{O} = \chi\). As the number of parameters \(D\) turns large, both the 2nd and 3rd terms will grow linearly w.r.t. \(D\), meaning that they contribute positively to the model complexity. Interestingly, the fourth term is a “negative complexity”. Regard \(\frac{1}{N \varepsilon_2^2}\) and \(\varepsilon_1\) as small positive values. The fourth term essentially is a log-ratio from the observed FIM to the true FIM. For small models, they coincide, because the sample size \(N\) is large based on the model size. In this case, the effect of this term is minor. For DNNs, the sample size \(N\) is very limited based on the huge model size \(D\). Along a dimension \(\theta_i\), \(3(\theta)\) is likely to be singular as stated in proposition 2, even if \(I\) has a very small positive value. In this case, their log-ratio will be negative. Therefore, the razor \(\mathcal{O}\) favors DNNs with their Fisher-spectrum clustered around 0.

In fig. 2, model C displays the concepts of a DNN, where there are many good local optima. The performance is not sensitive to specific values of model parameters. On the lightlike neuromanifold \(\mathcal{M}\), there are many directions that are very close to being lightlike. When a DNN model varies along these directions, the model slightly changes in terms of \(I(\theta)\), but their prediction on the samples measured by \(3(\theta)\) are invariant. These directions count negatively towards the complexity, because these extra freedoms (dimensions of \(\theta\)) occupy almost zero volume in the geometric sense, and are helpful to give a shorter code to future unseen samples.

To obtain a simpler expression, we consider the case that \(I(\theta) \equiv I(\hat{\theta})\) is both constant and diagonal in the interested region defined by eq. (25). In this case, \[
\log V \approx \frac{D}{2} \log 2\pi + D \log \varepsilon_2 + \frac{1}{2} \log |I(\hat{\theta}) + \varepsilon_1 I|. \tag{32}
\]
On the other hand, as $D \to \infty$, the spectrum of the FIM $I(\theta)$ will follow the density $\rho_I(\lambda)$. We plug these expressions into eq. (31), discard all lower-order terms, and get a simplified version of the razor

$$O \approx -\log p(X | \hat{\theta}) + \frac{D}{2} \log N + \frac{D}{2} \int_0^\infty \rho_I(\lambda) \log \left( \lambda + \frac{1}{N \varepsilon^2} \right) d\lambda,$$

(33)

where $\rho_I$ denotes the spectral density of the Fisher information matrix.

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