On the Power-Law Spectrum in Deep Learning: A Bridge to Protein Science

Zeke Xie 1  Qian-Yuan Tang 2  Yunfeng Cai 1  Mingming Sun 1  Ping Li 1

Abstract
It is well-known that the Hessian matters to optimization, generalization, and even robustness of deep learning. Recent works empirically discovered that the Hessian spectrum in deep learning has a two-component structure that consists of a small number of large eigenvalues and a large number of nearly-zero eigenvalues. However, the theoretical mechanism behind the Hessian spectrum is still absent or under-explored. We are the first to theoretically and empirically demonstrate that the Hessian spectrums of well-trained deep neural networks exhibit simple power-law distributions. Our work further reveals how the power-law spectrum essentially matters to deep learning: (1) it leads to low-dimensional and robust learning space, and (2) it implicitly penalizes the variational free energy, which results in low-complexity solutions. We further used the power-law spectral framework as a powerful tool to demonstrate multiple novel behaviors of deep learning. Interestingly, the power-law spectrum is also known to be important in protein, which indicates a novel bridge between deep learning and protein science.

1. Introduction
It is well-known that the Hessian matters to optimization, generalization, and even robustness of deep learning (Li et al., 2020; Ghorbani et al., 2019; Zhao et al., 2019; Jacot et al., 2019; Byrd et al., 2011). Deep learning usually finds flat minima that generalize well (Hochreiter & Schmidhuber, 1995; 1997). The Hessian is one of the most important measures of the minima flatness and directly relates to generalization in deep learning (Hoffer et al., 2017; Neyshabur et al., 2017; Dinh et al., 2017; Wu et al., 2017; Tsuzuku et al., 2020). Jiang et al. (2019) reported that minima-flatness-based generalization bound is still the most reliable metric in extensive experiments. Wu et al. (2017) reported that the low-complexity solutions that generalize well have a small norm of Hessian matrix with respect to model parameters. Yao et al. (2018) reported that the spectrum of the Hessian closely connects to large-batch training and adversarial robustness.

A number of works empirically studied the Hessian in deep neural networks. Some papers (Sagun et al., 2016; 2017; Wu et al., 2017) empirically observed that, in the context of deep learning, most eigenvalues of the Hessian are nearly zero, while a small number of eigenvalues are large. Sankar et al. (2021) revealed that the layerwise Hessian spectrum is similar to the entire Hessian spectrum. However, the theoretical mechanism behind the Hessian is still absent or under-explored.

Motivation. Why does the Hessian spectrum consist of a small number of large eigenvalues and a large number of nearly zero eigenvalues? Does an elegant mathematical structure hide behind the Hessian spectrum? Inspired by the lessons from proteins, our work provides a novel tool to understand and analyze deep learning from a spectral perspective.

Contributions. This paper mainly has three contributions.

1. First, to the best of our knowledge, we are the first to empirically discover and mathematically model the power-law Hessian spectrum in deep learning. We theoretically formulated a novel maximum entropy interpretation for explaining the power-law spectrum.

2. Second, we propose a framework of power-law spectral analysis for deep learning. We not only reveal how the power-law spectrum explains the theoretical origin of striking findings but also empirically demonstrate multiple novel behaviors of deep learning.

3. Third, we surprisingly discover that proteins, which are considered as the building blocks of life, also have a power-law spectrum. The power-law spectrums in proteins are natural results of protein evolution, which requires high functional accuracy and mutational robustness for surviving. This indicates a novel theoretical bridge between deep learning and protein science.
2. The Power-Law Spectrum

In this section, we reveal that the Hessian spectrums of well-trained deep neural networks have a simple power-law structure. We also show how to theoretically derive the power-law structure in the context of deep learning.

**Notations.** We denote the training dataset as \( \{(x, y)\} = \{(x_j, y_j)\}_{j=1}^N \) drawn from the data distribution \( S \), the \( n \) model parameters as \( \theta \) and the loss function over one data sample \( \{(x_j, y_j)\} \) as \( l(\theta, x_j, y_j) \). For simplicity, we further denote the training loss as \( L(\theta) = \frac{1}{N} \sum_{j=1}^N l(\theta, x_j, y_j) \). We write the descending ordered eigenvalues of the Hessian \( H \) as \( \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \) and denote the spectral density function as \( p(\lambda) \).

**Empirical evidence of the power-law Hessian spectrum.** Recent papers studied the Hessian but failed to reveal its elegant mathematical structure. For understanding the distribution of the Hessian spectrum better, we first visualize the Hessian spectrum of a well-trained neural network and a randomly initialized neural network by using the Lanczos algorithm (Meurant & Strakoš, 2006; Yao et al., 2020) to estimate the eigenvalues and spectral densities. In Figure 1, we display the top 6000 eigenvalues and their corresponding rank order. Both axes are log-scale. And we surprisingly discover an approximately straight line fits the Hessian spectrum of the well-trained neural network surprisingly well, except that a small number of outliers (~10) slightly deviate from the fitted straight line. To the best of our knowledge, this fitted straight line was not empirically discovered or theoretically discussed by previous papers in deep learning.

However, we surprisingly find that similar well-fitted straight lines have been reported and widely discussed as the power-law distribution in neuroscience (Stringer et al., 2019) and biology (Reuveni et al., 2008; Tang & Kaneko, 2020). This is exactly our motivation to further verify and study the power-law structure of the Hessian spectrum in the context of deep learning. Interestingly and fortunately, we verify the elegant power-law structure indeed exists in well-trained deep neural networks just like bioactive proteins. In contrast, random neural networks have no such a power-law structure, just like deactivated (denatured or unfolded) proteins. It means random neural networks, as well as deactivated proteins, have no functional ability on the given task. We will discuss the deep connection in Section 4.

The well-fitted straight line means that the observed distribution of the Hessian eigenvalues of trained neural networks approximately obey a power-law distribution,

\[
p(\lambda) = Z_c^{-1} \lambda^{-\beta},
\]

where \( Z_c \) is the normalization factor. The observed eigenvalues can be considered as \( n \) samples from the power-law distribution \( p(\lambda) \). We may also use a corresponding finite-sample power law for describing the observed law as

\[
f_k = \frac{\lambda_k}{\text{Tr}(H)} = \frac{Z_d^{-1}}{k^{-\frac{1}{\beta}},}
\]

where \( f \) is the trace-normalized eigenvalue, \( k \) is the rank order, the trace \( \text{Tr}(H) = \sum_{k=1}^n \lambda_k \), and \( Z_d = \sum_{k=1}^n k^{-\frac{1}{\beta}} \) is the normalization factor for the finite-sample power law. Note that the finite-sample power law is also called Zipf’s law. This can also be equivalently written as

\[
\lambda_k = \lambda_1 k^{-s},
\]

if we let \( s = \frac{1}{\beta-1} \) denote the power exponent of Zipf’s law. The empirical power-law spectrums suggest that the estimated \( \beta \) is close to 2 and the estimated \( s \) is close to 1.

**Deriving the power-law spectrum from maximum entropy principle.** The maximum entropy principle (Guiasu & Shenitzer, 1985), also named the maximum entropy prior, states that the probability distribution which best represents the current state of knowledge about a system is the one with the highest entropy. This principle indicates that if we have no prior knowledge for suspecting one state over any other, then all states must be considered equally likely.

We start our Hessian spectral theoretical analysis by maximum entropy in deep learning. The log space volume is often regarded a kind of entropy in statistical physics (Visser, 2013). Note that flat minima have larger space volume reflected by \( \det(H^{-1}) \). It means maximizing the minima space volume for better generalization may be regarded as a kind of entropy maximization principle. Following Visser (2013), we may explicitly write the volume entropy as

\[
S_{\text{vol}} = -\log \det(H) = \int p(\lambda) \log \lambda d\lambda
\]

and the spectral entropy as

\[
S_p = -\int p(\lambda) \log p(\lambda) d\lambda,
\]

which is the entropy of the spectral density distribution. Considering the principle of maximum entropy with the two kinds of entropy, we need to maximize the total entropy with the spectral density normalization constraint

\[
S_{\text{total}} = -\int p(\lambda) \log p(\lambda) d\lambda - \beta_{\text{vol}} \int p(\lambda) \log \lambda d\lambda
\]

\[
- \beta_{\text{norm}}(\int p(\lambda) d\lambda - 1),
\]

where \( S_{\text{total}} = S_p + \beta_{\text{vol}} S_{\text{vol}} \) and \( \beta_{\text{norm}} \) is a Lagrange multiplier. To find the optimal distribution \( p^*(\lambda) \) that maximizes the total entropy, we require the following

\[
\frac{\partial S_{\text{total}}}{\partial p(\lambda)} = -\log p(\lambda) - \beta_{\text{vol}} \log \lambda - \beta_{\text{norm}} = 0.
\]
Thus, the optimal distribution $p^*(\lambda)$ can be solved as
\[
p^*(\lambda) = e^{-\beta_{\text{norm}} \lambda^{-\beta_{\text{vol}}}}.
\] (8)

This has an amazingly similar form to our empirical result Equation (1) with $\beta_{\text{norm}} = \log Z_c$ and $\beta = \beta_{\text{vol}}$.

We successfully derived the power-law structure of the Hessian spectrum from two simple maximum entropy principles with the spectral density normalization constraint. It roughly means that simple rules can almost explain the power-law Hessian spectrum in deep learning. The spectrums have much simpler structures than previous work expected.

The Kolmogorov-Smirnov Goodness-of-fit Test. Following Alstott et al. (2014), our work used Maximum Likelihood Estimation (MLE) (Myung, 2003) for estimating the parameter $\beta$ of the fitted power-law distributions and the Kolmogorov-Smirnov Test (KS Test) (Massey Jr, 1951; Goldstein et al., 2004) for statistically testing the goodness of the fit. The KS test statistic is the KS distance $d_{ks}$ between the hypothesized (fitted) distribution and the empirical data, which measures the goodness of fit.

According to the practice of KS Test (Massey Jr, 1951), we state the null hypothesis that the tested spectrum is not power-law. We state the alternative hypothesis, called the power-law hypothesis, that the tested spectrum is power-law. If $d_{ks}$ is higher than the critical value $d_c$ at the $\alpha = 0.05$ significance level, we would accept the null hypothesis. Or we would reject the null hypothesis and accept the power-law hypothesis. We leave the details and test results, including KS test critical values and KS distance, in Appendix A.

Thus, when we say that a spectrum is (approximately) power-law in this paper, we mean that the KS test supports to accept the power-law hypothesis rather than the null hypothesis. Our results show that, we accept the null hypothesis for random neural networks and accept the power-law hypothesis for well-trained neural networks. Moreover, when the power-law hypothesis holds as we discover in this paper, the KS distance is usually significantly smaller than the critical value $d_c$. For simplicity, the default $\alpha = 0.05$ significance level is abbreviated in the following.

Following related work on the Hessian of neural networks (Thomas et al., 2020), our empirical analysis and statistical tests mainly focused on the top ($\sim 1000$) large eigenvalues rather than some minimal cutoff value $\lambda_{cutoff}$ for three reasons. First, focusing on relatively large values is very reasonable and common in various fields’ power-law studies, as real-world distributions typically follow power laws only after/large than some cutoff values (Clauset et al., 2009) for ensuring the convergence of the probability distribution. Second, researchers are usually more interested in significantly large eigenvalues which contributes more to the minima sharpness or generalization bound (Thomas et al., 2020). Third, empirically estimating a large number of nearly zero eigenvalues is very inaccurate and expensive.

Related Works. A number of related works theoretically analyzed the spectral distribution of the Hessian in deep learning. However, previous papers failed to theoretically or empirically model the observed spectral distribution in practical deep learning. Pennington & Bahri (2017) introduced an analytical framework from random matrix theory and reported that the shape of the spectrum depends strongly on the energy and the overparameterization parameter, $\phi$, which measures the ratio of parameters to data points. However, Pennington & Bahri (2017) mainly evaluated single-hidden-layer networks, which limits the scope of the conclusion. A followup work (Pennington & Worah, 2018) focused on a single-hidden-layer neural network with Gaussian data and weights in the limit of infinite width. Obviously, its theoretical and empirical analysis is far from practical deep models. Jacot et al. (2019) analyzed the limiting spectrum of the Hessian in neural networks with infinite width. Liao & Mahoney (2021) studied the Hessian spectrums of more realistic nonlinear models. While a number of previous papers studied the Hessian spectrum, they failed to empirically discover the simple but important power-law structure and
We try to mathematically answer this question by studying Ari et al. (2018) empirically observed that deep learning (via approximately matching the Hessian eigengaps. We define the i-th eigengap as

\[ \delta_k = \left\langle u_k, \tilde{u}_k \right\rangle \]

and its corresponding perturbed eigenvector is \( \tilde{u}_k \). To measure the robustness of space’s dimensions, we directly apply Theorem 1, a useful variant of Davis-Kahan Theorem (Yu et al., 2015), to the Hessian in deep learning, which states that the eigenspace (spanned by eigenvector) robustness can be well bounded by the corresponding eigengap.

**Empirical analysis of the decaying Hessian eigengaps.** The empirical study about the Hessian eigengaps is missing in previous papers. Our experiments filled this gap. Our experiments show that top eigengaps dominate others in deep learning similarly to eigenvalues. We further empirically verified the approximate power-law distribution of the eigengaps in Figure 2. Moreover, the observation that the power exponent of eigengaps is larger than the power exponent of eigenvalues by \( \sim 1 \) even fully matches our theoretical result by comparing Equations (2) and (10).

Note that the existence of top large eigenvalues does not necessarily indicate their gaps are also statistically large. Previous papers revealed that top eigenvalues dominate others but did not reveal if top eigengaps dominate others in deep learning. Fortunately, we theoretically and empirically demonstrate that both eigenvalues and eigengaps decay, obeying a power law as the rank order increase. Eigengaps even decay faster than eigenvalues due to the larger magnitude of the power exponent. We will show that this is the foundation of learning space robustness in deep learning.

**Eigengaps Bound Learning Space Robustness.** Based on the well-known Davis-Kahan \( \sin(\Theta) \) Theorem (Davis & Kahan, 1970), we use the angle of the original eigenvector \( u_k \) and the perturbed eigenvector \( \tilde{u}_k \), namely \( \left\langle u_k, \tilde{u}_k \right\rangle \), to measure the robustness of space’s dimensions. We directly apply Theorem 1, a useful variant of Davis-Kahan Theorem (Yu et al., 2015), to the Hessian in deep learning, which states that the eigenspace (spanned by eigenvector) robustness can be well bounded by the corresponding eigengap.

**Theorem 1 (Eigengaps Bound Eigenspace Robustness (Yu et al., 2015)).** Suppose the true Hessian is \( H \), the perturbed Hessian is \( \tilde{H} = H + \epsilon M \), the i-th eigenvector of \( H \) is \( u_i \), and its corresponding perturbed eigenvector is \( \tilde{u}_i \). Under the conditions of Davis-Kahan Theorem, we have

\[ \sin(\left\langle u_k, \tilde{u}_k \right\rangle) \leq \frac{2\epsilon \|M\|_{op}}{\min(\lambda_{k-1} - \lambda_k, \lambda_k - \lambda_{k+1})}, \]

where \( \|M\|_{op} \) is the operator norm of \( M \).

As we have a small number of large eigengaps corresponding to the large eigenvalues, the corresponding learning space robustness has a tight upper bound. For example, given the power-law eigengaps in Equation (10), the upper bound of

\[ \delta_k = \Tr(H) Z_d^{-1} (k+1)^{-(s+1)} \]

under the empirical approximation \( s \approx 1 \). The power exponent \( s + 1 \) is larger than the one in Equation (2) by 1.

3. Spectrum Matters to Deep Learning

In this section, we develop a Hessian Spectral Theory for deep learning and reveal how the power-law spectrum critically affects deep learning in multiple aspects. The discovered power-law structure provides novel insights and helps understand important properties of deep learning.

3.1. Robust and Low-Dimensional Learning Space

Deep learning happens in a low-dimensional space. Gur-Ari et al. (2018) empirically observed that deep learning (via SGD) mainly happens in a low-dimensional space during the whole training process. Ghorbani et al. (2019) studied and reported that, throughout the optimization process, large isolated eigenvalues rapidly appear in the spectrum, along with a surprising concentration of the gradient in the corresponding eigenspace. Xie et al. (2021b) theoretically demonstrated that the learning space is a low-dimensional subspace spanned by the eigenvectors corresponding to large eigenvalues of the Hessian, because SGD diffusion mainly happens along these principal components. Note that the low-dimensional learning space implicitly reduces deep models’ complexity. However, existing work cannot explain why the low-dimensional learning space is robust during training. In this paper, robust space means that the space’s dimensions are robust or table during training.

We try to mathematically answer this question by studying the Hessian eigengaps. We define the i-th eigengap as \( \delta_k = \lambda_k - \lambda_{k+1} \). According to Equation (2), we have \( \delta_k \) approximately meeting

\[ \delta_k = \Tr(H) Z_d^{-1} (k+1)^{-(s+1)} \approx \lambda_k \left[ 1 - \left( \frac{k}{k+1} \right)^s \right]. \]
eigenvector robustness can be written as
\[
\sup \sin(u_k, \tilde{u}_k) = \frac{2\epsilon\|M\|_{op}(k + 1)^{s+1}}{\lambda_1},
\]
which is relatively tight for top dimensions (small \(k\)) but becomes very loose for tail dimensions (large \(k\)). A similar conclusion also holds given Equation (9). As \(s \approx 1\) suggests, the experimental results in Figure 2 also well supports that the upper bound of \(k = 10\) is \(10^4\) times the upper bound of \(k = 1000\). This indicates that non-principal components’ space can be highly unstable during training, because \(\delta_k\) can decay to nearly zero for a large \(k\). To the best of our knowledge, we are the first to mathematically prove that the robustness of low-dimensional learning space directly depends on the eigengaps of the Hessian \(H\).

3.2. The Variational Bayesian Interpretation

In this subsection, we discuss SGD and the power-law spectrum in the Variational Bayesian framework.

Variational Bayesian Inference. Performing Bayesian inference on a neural network requires the posterior distribution of the network weights given the dataset \(S\). Unfortunately, for most neural networks the true Bayesian posterior \(P(\theta | S)\) is intractable analytically. Variational Bayesian inference addresses this problem by approximating the Bayesian posterior \(P(\theta | S)\) by a more tractable and practical distribution \(Q(\theta | \tau)\), which is not a Bayesian posterior but some posterior distribution that we specify or given by a algorithm. The approximation will be fitted if the posterior \(Q(\theta | \tau)\) may well minimize the variational free energy
\[
\mathcal{F} = E_{\theta \sim Q}[L(\theta)] + KL[Q||P],
\]
where \(KL(Q||P)\) denotes the Kullback–Leibler divergence from \(P\) to \(Q\).

Following Graves (2011), the first term \(E_{\theta \sim Q}[L(\theta)]\) is the error loss, since this term directly depends on the training errors; the second term \(KL[Q||P]\) is the complexity loss, since this term measures the cost of “describing” the network weights to the receiver in the framework of the Minimum Description Length (MDL) (Barron et al., 1998; Honkela & Valpola, 2004; Grünwald, 2007). We may also interpret \(\mathcal{F}\) as a MDL loss (Graves, 2011). A general belief is that, holding accuracy constant, the best model is the one with the shortest MDL (Hinton & Camp, 1993).

Mandt et al. (2017) demonstrated that SGD may approximately perform Bayesian inference. If we consider \(Q\) as the posterior distribution produced by SGD, then how well does the SGD posterior minimize the variational free energy as well as the description length loss?

The SGD posterior analysis. In the following analysis, we focus on the posterior near minima and apply the second-order Taylor approximation in the local region as Assumption 1. Note that Assumption 1 is mild near minima and common in a large number of related works (Mandt et al., 2017; Zhang et al., 2019a; Neyshabur et al., 2017; Xie et al., 2021ab).

Assumption 1. The loss function around a minimum \(\theta^*\) can be approximately written as
\[
L(\theta) = L(\theta^*) + \frac{1}{2}(\theta - \theta^*)^\top H(\theta^*)(\theta - \theta^*).
\]

Mandt et al. (2017) demonstrated that, the SGD posterior in the local region around a minimum \(\theta^*\) is approximately a Gaussian distribution \(N(\theta^*, \Sigma_{sgd})\). This well-known result can be formulated as Theorem 2. We denote that \(C(\theta^*) = C\) in the following analysis.

Theorem 2 (The SGD posterior near a minimum (Mandt et al., 2017)). Suppose that Assumption 1 holds, the covariance near the minimum \(\theta^*\) is \(C(\theta^*)\), the dynamics is governed by continuous-time SGD. Then, in the long-time limit, the generated posterior \(Q\) near \(\theta^*\) is a Gaussian distribution \(N(\theta^*, \Sigma)\), where the \(\Sigma\) satisfies
\[
\Sigma H(\theta^*) + H(\theta^*)\Sigma = \eta C(\theta^*).
\]

Based on Jastrzkebski et al. (2017); Zhu et al. (2019); Xie et al. (2021b), the covariance \(C(\theta)\) is proportional to the Hessian \(H(\theta)\) and inverse to the batch size \(B\) near minima:
\[
C_{sgd}(\theta) \approx \frac{1}{B} H(\theta).
\]

Equation (13) has also been empirically verified by related papers (Xie et al., 2021b). By Equation (13) and Theorem 2, we may further express \(\Sigma_{sgd}\) as
\[
\Sigma_{sgd} = \frac{\eta}{2B} I, \tag{14}
\]

where \(I\) is the \(n \times n\) identity matrix. Thus, the SGD posterior \(Q\) near the minimum \(\theta^*\) is the Gaussian distribution \(N(\theta^*, \frac{n}{2B} I)\). Note that similar posterior analysis is widely used in related works (Mandt et al., 2017; He et al., 2019).

VARIATIONAL FREE ENERGY. On the other hand, the Bayesian prior posterior \(P\) near minimum \(\theta^*\) can be written as \(\mathcal{N}(\theta^*, \tau H^{-1})\), which \(\tau\) is a temperature hyperparameter. We note that, \(\tau = 1\) holds for the standard Bayesian posterior, while people sometimes use \(\tau \leq 1\) in Bayesian deep learning for better practical performance, called cold Bayesian posteriors (Wenzel et al., 2020).

Thus, \(KL[Q||P]\) can be written as
\[
KL[Q||P] = \frac{1}{2} \left[ \log \frac{\det(\Sigma_P)}{\det(\Sigma_Q)} + \text{Tr}(\Sigma_P^{-1}\Sigma_Q) \right] + \frac{1}{2}(\mu_Q - \mu_P)^\top \Sigma_P^{-1}(\mu_Q - \mu_P) - \frac{n}{2} \tag{15}
\]
where $\mu_\Omega = \mu_P = \theta^*$, $\Sigma_\Omega = \frac{\eta}{2B} I$, and $\Sigma_P = \tau H^{-1}$.

Then we have

$$
\text{KL}[Q \| P] = \frac{1}{2} \left[ \log \det \left( \frac{2B \tau}{\eta} H^{-1} \right) + \frac{\eta}{2B \tau} \text{Tr}(H) \right] - \frac{n}{2}
$$

$$
= -\frac{1}{2} \log \det(H) + \frac{\eta}{4B} \text{Tr}(H)
$$

$$
+ \frac{n}{2} \left[ \log 2B \tau - 1 \right].
$$

(16)

Given the expression of $\text{KL}[Q \| P]$ above, we may further write the variational free energy $\mathcal{F}$ as

$$
\mathcal{F} = L(\theta^*) + E_{\theta-Q}[L(\theta) - L(\theta^*)] + \text{KL}[Q \| P]
$$

$$
= L(\theta^*) - \frac{1}{2} \log \det(H) + \frac{\eta}{4B} \left( 1 + \frac{1}{\tau} \right) \text{Tr}(H)
$$

$$
+ \frac{n}{2} \left[ \log 2B \tau - 1 \right].
$$

(17)

**Discussion.** The variational free energy loss above includes four terms: (1) the training loss which is explicitly optimized by SGD during training, (2) a volume-entropy regularizer which penalizes the negative log Hessian determinant, (3) a regularizer which penalizes the Hessian trace, and (4) a term which is decided by hyperparameters and independent of training. Note that the power-law spectrum which explicitly optimizes the volume entropy $- \log \det(H)$ also penalizes the complexity loss in the variational free energy.

We also note that the regularization strength of the third term is usually ignorable compared to the second term, because $\frac{1}{2B}(1 + \frac{1}{\tau}) \ll 1$ generally hold in common settings. For example, we have $\frac{\eta}{4B} \approx 3.9 \times 10^{-6}$ for the common setting that $\eta = 0.001$ (after the final learning rate decay) and $B = 128$. Moreover, the true Bayesian posterior has $\tau = 1$. While the learning rate $\eta$ and batch size $B$ are the tunable hyperparameters, $\frac{1}{2B}(1 + \frac{1}{\tau})$ is much smaller than $\frac{1}{2}$ by five orders of the magnitude in the common settings. Thus, for simplicity, we may ignore the third Hessian-trace regularization term in practice due to the much stronger log Hessian determinant regularization term.

In summary, SGD itself explicitly optimizes the training loss, the power-law spectrum implicitly optimizes the second term, the third term is usually approximately ignorable in practical applications, and the fourth term is independent of training. Our theoretical analysis demonstrates that deep networks trained via SGD actually penalize the variational free energy loss as well as the description length effectively, which indicates the low-complexity solution in the Variational Bayesian framework (Beal, 2003; Rissanen, 2007; Blier & Ollivier, 2018). Note that the minimum description length implies the low-complexity solution and better generalization (Hinton & Camp, 1993; Grünwald, 2007; Blier & Ollivier, 2018). The spectrum-based analysis provides novel evidence for understanding good generalization in deep learning.

**4. A Bridge to Protein Science**

In this section, we discuss protein and how it inspired our discussions on the spectrums of neural networks.

As the basic building blocks of biological intelligence, proteins work as the main executors of various vital functions, including catalysis (enzyme), transportation (carrier proteins), defense (antibodies), and so on. The polypeptide chain made up of amino acid residues can fold into its native (energy-minimum) three-dimensional structure from a random coil. For most proteins, their “correct” native structures are essential to their functions. These structures (denote as $\vec{r}^0$) are not static. In contrast, they can perform their intrinsic dynamics due to the perturbations from the milieu. When external thermal noise act as force $\vec{\xi}$, the protein’s deformation $\Delta \vec{r} = \vec{r} - \vec{r}^0$ can be estimated as: $\Delta \vec{r} = H^{-1} \vec{\xi}$, where $H$ is the elasticity matrix, i.e., the Hessian of the potential energy landscape. Such a framework is known as the elastic network model of the proteins (Atilgan et al., 2001; Bahar et al., 2010). When take the external thermal noises $\vec{\xi}$ as the input variable, the deformation $\Delta \vec{r}$ can be recognized as the output of a trained network, and the native structure $\vec{r}^0$ encoding the elastic network corresponds to the parameters of the network.

**Proteins as accurate and robust learners.** It is worth noting that, in a long timescale, the native structure (network parameter) $\vec{r}^0$ has been gradually shaped by evolution. Due to random mutations, the native structure (energy-minimum point) and corresponding elastic network have varied. Thus, protein evolution can be recognized as an optimization process of the network parameters (Tang & Kaneko, 2021). With the second-order Taylor approximation near a minimum, for a given native structure $\vec{r}^0$, the potential energy can be calculated as:

$$
E(\vec{r}^0) = E(\vec{r}^*) + \frac{1}{2} (\vec{r}^0 - \vec{r}^*)^\top H(\vec{r}^*)(\vec{r}^0 - \vec{r}^*),
$$

(18)

in which $\vec{r}^*$ denote the reference structure, a selected ancestral structure in the evolution, and $H(\vec{r}^*)$ is its corresponding Hessian. In this way, the evolution of a protein become comparable to the training of artificial neural networks. The potential energy $E$ corresponds to the loss function $L$, while native structure $\vec{r}^0$ corresponds to the model parameters $\theta$.

**1) Accuracy.** Proteins can respond with high susceptibility when perturbed by the environment, and some can undergo significant structural changes (Tang et al., 2017). The noise-induced motions are highly anisotropic, with amino acid residues moving collectively in specific directions. These movements are usually related to the protein functions (Bahar et al., 2010). It is analogous to the model’s generalization ability which describes how a model (protein) can deal with new data (different external noises) and make accurate predictions (specific functional dynamics).
(2) **Robustness.** In protein evolution, it is the functions of proteins that act as constraints, so essential functions must withstand most mutations (Guo et al., 2004; Tang & Kaneko, 2021). It is observed that, when the environment is stable, organisms tend to evolve in a convergent direction (Sato & Kaneko, 2020; Sakata & Kaneko, 2020). Upon recognizing the protein as a learner, it is remarkable that the gradients (direction of evolution) on the loss landscape remain relatively stable. During evolution, most mutations do not affect the direction of the principal-component vectors (or the low-dimensional subspaces spanned by these vectors) related to the functions of the protein. This idea aligns with the discussions on the eigengaps in previous sections.

**Power law and criticality.** We take a protein assembly (shown in Figure 3a) as an example to conduct normal mode analysis and obtain the vibration spectrum. This calculation is based on the elastic network model (See Appendix C). The result is shown in Figure 3b. We evaluate 9166 kinds of proteins in Section 5. While recent studies (Reuveni et al., 2008; Tang & Kaneko, 2020; Tang et al., 2020) implicitly or explicitly suggested that the vibration spectrum of proteins exhibits a power-law distribution, we are the first to conduct large-scale statistical tests on the power-law spectrums for protein. The power-law behaviors suggest the parallels between protein evolution and deep learning. Interestingly, similar power laws were observed in various kinds of other natural systems, including brains, bird flocks, insect swarms, and so on (Munoz, 2018). In statistical physics, power laws act as the hallmark of “critical point” between ordered (robustness) and disordered (plasticity) states.

5. Discussion and Empirical Analysis

In this section, we present extensive experimental results for exploring the power-law spectrums in deep learning.

**Model:** LeNet (LeCun et al., 1998), Fully Connected Networks (FCN), and ResNet18 (He et al., 2016). **Dataset:** MNIST (LeCun, 1998), Fashion-MNIST (Xiao et al., 2017), CIFAR-10/100 (Krizhevsky & Hinton, 2009), and non-image Avila (De Stefano et al., 2018).

**1. Optimization and Generalization.** Figure 4 discovered that the power-law spectrum consistently holds for various popular optimizers, such as SGD, Vanilla SGD, Adam (Kingma & Ba, 2015), AMSGrad (Reddi et al., 2019), AdaBound (Luo et al., 2019), Yogi (Zaheer et al., 2018), RAdam (Liu et al., 2019), Adai (Xie et al., 2020b), PNM (Xie et al., 2021c), Lookahead (Zhang et al., 2019b), and DiffGrad (Dubey et al., 2019), as long as the optimizers can train neural networks well.

We find that the slope magnitude \( \hat{s} \) of the fitted straight line may serve as a nice indicator of minima sharpness and a predictor of test performance. It is common to measure minima sharpness by the largest Hessian eigenvalue or the Hessian trace. A smaller \( \hat{s} \) highly correlates to a smaller largest eigenvalue and a smaller trace in Figure 14 of Appendix D. The observation also holds on CIFAR-10 in Figures 13 and 15 of Appendix D.

**2. Evaluating 9166 kinds of Proteins.** Surprisingly, we observed \( \hat{s} \approx 1 \) for the protein in Figure 3 and in the spectrums of total 9166 kinds of protein molecules from the Protein Data Bank (PDB) (Berman et al., 2000). Each of the protein molecule has \( 100 \leq N_{AA} \leq 2000 \) amino acid residues. All of the protein spectrums successfully passed the power-law KS tests with \( mean(\hat{s}) = 1.045 \) (\( mean(\hat{\beta}) = 1.975 \)). The approximation \( \hat{s} \approx 1 \) holds even better for large proteins in terms of the mean and the standard error, shown in Table 1. We conjecture there may exist some universal underly mechanism for deep learning and protein.

**3. Overparameterization.** Figure 5 shows that the power-law spectrum holds well in overparameterized models, but disappears in underparameterized models. Overparameterization is necessary for the power-law spectrum in deep

**Figure 3.** (a) The cartoon illustration of human deoxyhemoglobin tetramer (PDB code: 4HHB). (b) The vibrational spectrum of the protein’s elastic network. The estimated power exponent (slope magnitude) \( \hat{s} = 0.992 (\hat{\beta} = 2.008 \pm 0.032) \), which is very close to the estimated power exponent in deep learning.

**Figure 4.** The power-law spectrums hold across optimizers. Moreover, the slope magnitude \( \hat{s} \) is an indicator of minima sharpness and a predictor of test performance. **Model:** LeNet. **Dataset:** MNIST.

**Table 1.** The estimated \( \hat{s} \) for various sized proteins.

| Slope | SLOPE \( \leq 3N_{AA} \leq 1000 \) | SLOPE \( 1000 \leq 3N_{AA} \leq 3000 \) | SLOPE \( 3000 \leq 3N_{AA} \leq 6000 \) |
|-------|----------------|----------------|----------------|
| \( \hat{s} \) | 1.050 \( \pm 0.175 \) | 1.041 \( \pm 0.119 \) | 1.002 \( \pm 0.084 \) |
learning, while proteins are also high-dimensional. It will be interesting to study the theoretical origin and transition of overparameterization and underparameterization in future.

4. Batch Size. We discover the three significantly different phases for large-batch training in Figure 6. First, in Phase I ($B \leq 640$), moderately large-batch ($B = 512$) training indeed finds sharper minima than small-batch ($B = 128$) training, while the power-law spectrum still holds well. Power laws may guarantee that the top eigenvalues of large-batch trained networks are all larger than the corresponding eigenvalues of small-batch trained networks. The main challenge of large-batch training in Phase I is consistent with the common belief that large-batch training suffers from sharp minima and, thus, leads to bad generalization (Hoffer et al., 2017; Keskar et al., 2017). The batch size well correlates with minima sharpness measured by $s$.

Second, in Phase II ($768 \leq B \leq 50000$), the spectrum of large-batch ($B = 1024$) trained networks does not exhibit power laws but is visually similar to the spectrum of underparameterized models in Figure 5. In Phase II, large-batch trained overparameterized models behave like underparameterized models from a spectral perspective, and, thus, can lead to bad generalization. The phase transition from Phase I to Phase II occurs in a narrow range of $640 < B < 768$.

Third, in Phase III ($B \sim 60000$), extremely large-batch training ($B = 60000$) cannot optimize the training loss well and, obviously, finds the Hessian spectrum similarly to random initialized neural networks. Phase III indicates that, sometimes, bad convergence rather than sharp minima can become the main performance bottleneck in large-batch training (Xie et al., 2020a), when the batch size is too large.

To the best of our knowledge, we are the first to report Phase II, while Phase III was theoretically predicted by Xie et al. (2020a) but lacked direct empirical evidence before.

5. Learning with Noisy Labels. Learning with noisy labels (Han et al., 2020) has become a hot topic. Figure 7 shows that label noise makes the spectrum on the noisy training dataset less power-law, while it breaks the power-law structure of the spectrums on the clean test dataset. In contrast, in the absence of noisy labels, the power-law spectrums exist on both the training dataset and the test dataset.

6. Supplementary Results. In Appendix D, we further discussed various interesting empirical results, including ResNet18, Random Labels, and Avila.

6. Conclusion

In this paper, we report the power-law spectrum in deep learning. Inspired by statistical physical theory (Visser, 2013) and protein theory (Tang et al., 2020), we successfully formulated a novel maximum entropy interpretation. The power-law spectrums provide us with a powerful tool to understand and analyze deep learning, theoretically and empirically. We not only presented novel analysis on learning space robustness and variational free energy, but also empirically demonstrate multiple novel behaviors of deep learning beyond previous studies. Moreover, our large-scale study on proteins reveals the deep connections to deep learning. We believe our work will inspire more theories and empirical advancements on both deep learning and protein in the future.
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The Power-Law Spectrum

Table 2. The Table of Kolmogorov-Smirnov Test Critical Values (Significance Level), which was first reported in Massey Jr (1951). If the KS distance \( d_{ks} \) is lower than a critical value, such as \( 1.36 \sqrt{K} \), we would reject the null hypothesis and accept the power-law hypothesis at the \( \alpha = 0.05 \) significance level. Note that \( K \) is the number of tested eigenvalues.

| Sample size | \( \alpha = 0.2 \) | \( \alpha = 0.15 \) | \( \alpha = 0.1 \) | \( \alpha = 0.05 \) | \( \alpha = 0.01 \) |
|-------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| \( K > 35 \) | \( 1.07 \sqrt{K} \) | \( 1.14 \sqrt{K} \) | \( 1.22 \sqrt{K} \) | \( 1.36 \sqrt{K} \) | \( 1.63 \sqrt{K} \) |
| \( K = 50 \) | 0.151 | 0.161 | 0.173 | 0.192 | 0.231 |
| \( K = 1000 \) | 0.0338 | 0.0360 | 0.0386 | 0.0430 | 0.0515 |

A. Kolmogorov-Smirnov Goodness-of-Fit Test

In this section, we introduce how to conduct the Kolmogorov-Smirnov Goodness-of-Fit Test for the self-containedness purpose.

As we mentioned above, our work used Maximum Likelihood Estimation (MLE) (Myung, 2003; Clauset et al., 2009) for estimating the parameter \( \beta \) of the fitted power-law distributions and the Kolmogorov-Smirnov Test (KS Test) (Massey Jr, 1951; Goldstein et al., 2004) for statistically testing the goodness of the fit. The KS test statistic is the KS distance \( d_{ks} \) between the hypothesized (fitted) distribution and the empirical data, which measures the goodness of fit. Mathematically, the KS distance is defined as

\[
d_{ks} = \sup_{\lambda} |F^*(\lambda) - \hat{F}(\lambda)|,
\]

where \( F^*(\lambda) \) is the hypothesized cumulative distribution function and \( \hat{F}(\lambda) \) is the empirical cumulative distribution function based on the sampled data (Goldstein et al., 2004). The estimated power exponent via MLE (Clauset et al., 2009) can be written as

\[
\hat{\beta} = 1 + K \left[ \sum_{i=1}^{K} \ln \left( \frac{\lambda_i}{\lambda_{\text{cutoff}}} \right) \right]^{-1},
\]

where \( K \) is the number of tested samples and we set \( \lambda_{\text{cutoff}} = \lambda_k \). We note that the Powerlaw library (Alstott et al., 2014) provides a convenient tool to compute the KS distance, \( d_{ks} \), and estimate the power exponent.

According to the practice of Kolmogorov-Smirnov Test (Massey Jr, 1951), we state the null hypothesis that the tested spectrum is not power-law. We state the alternative hypothesis, called the power-law hypothesis, that the tested spectrum is power-law. If \( d_{ks} \) is higher than the critical value \( d_c \) at the \( \alpha = 0.05 \) significance level, we would accept the null hypothesis. In contrast, if \( d_{ks} \) is lower than the critical value \( d_c \) at the \( \alpha = 0.05 \) significance level, we would reject the null hypothesis and accept the power-law hypothesis. We display the critical values in Table 2.

We conducted the KS tests for all of our studied spectrums. We display the KS test statistics and the estimated power exponents \( \hat{\beta} \) with standard errors \( \sigma \) as well as the corresponding \( \hat{s} \) in Tables 3, 4, 5, 6, and 7. In the tables, we take the base hyperparameter setting in Appendix B as the default setting. For better visualization, we color accepting the power-law hypothesis in blue and color accepting the null hypothesis (and the cause) in red.

B. Experimental Settings

B.1. Models, Datasets, and Optimizers

Models: LeNet (LeCun et al., 1998), Fully Connected Networks (FCN), and ResNet18 (He et al., 2016). Particularly, we used one-layer FCN, two-layer FCN, four-layer FCN, which have 100 neurons for each hidden layer and use ReLu activations.

Datasets: MNIST (LeCun, 1998), Fashion-MNIST (Xiao et al., 2017), CIFAR-10/100 (Krizhevsky & Hinton, 2009), and non-image Avila (De Stefano et al., 2018).

Optimizers: SGD, Vanilla SGD, Adam (Kingma & Ba, 2015), AMSGrad (Reddi et al., 2019), AdaBound (Luo et al., 2019), Yogi (Zaheer et al., 2018), RAdam (Liu et al., 2019), Adai (Xie et al., 2020b), PNM (Xie et al., 2021c), Lookahead (Zhang et al., 2019b), and DiffGrad (Dubey et al., 2019).
Table 3. The Kolmogorov-Smirnov statistics of LeNet on MNIST and Fashion MNIST. The estimated power exponent $\hat{\beta}$ and slope magnitude $\hat{s}$ are also displayed.

| Dataset      | Model      | Training  | Sample size | Setting | $d_{ks}$ | $d_s$ | Power-Law | $\hat{\beta} \pm \sigma$ | $\hat{s}$ |
|--------------|------------|-----------|-------------|---------|----------|------|-----------|------------------------|--------|
| MNIST        | LeNet      | Random    | 1000        | -       | 0.0796   | 0.0430| No        | 1.991 ± 0.031         | 1.009  |
| MNIST        | LeNet      | SGD       | 1000        | -       | 0.00900  | 0.0430| Yes       | 1.914 ± 0.029         | 1.094  |
| MNIST        | LeNet      | Vanilla SGD | 1000    | -       | 0.0103   | 0.0430| Yes       | 1.873 ± 0.028         | 1.145  |
| MNIST        | LeNet      | Adam      | 1000        | -       | 0.00962  | 0.0430| Yes       | 1.845 ± 0.027         | 1.184  |
| MNIST        | LeNet      | AMSGrad   | 1000        | -       | 0.00987  | 0.0430| Yes       | 1.904 ± 0.029         | 1.106  |
| MNIST        | LeNet      | AdaBound  | 1000        | -       | 0.00889  | 0.0430| Yes       | 1.834 ± 0.026         | 1.198  |
| MNIST        | LeNet      | Yogi      | 1000        | -       | 0.00966  | 0.0430| Yes       | 1.889 ± 0.028         | 1.125  |
| MNIST        | LeNet      | RAdam     | 1000        | -       | 0.0164   | 0.0430| Yes       | 1.892 ± 0.028         | 1.181  |
| MNIST        | LeNet      | Adai      | 1000        | -       | 0.00101  | 0.0430| Yes       | 1.846 ± 0.027         | 1.119  |
| MNIST        | LeNet      | PNM       | 1000        | -       | 0.0127   | 0.0430| Yes       | 1.834 ± 0.026         | 1.198  |
| MNIST        | LeNet      | Lookahead | 1000        | -       | 0.00101  | 0.0430| Yes       | 1.982 ± 0.031         | 1.018  |
| MNIST        | LeNet      | DiffGrad  | 1000        | -       | 0.0105   | 0.0430| Yes       | 1.834 ± 0.026         | 1.198  |
| MNIST        | LeNet      | SGD       | 1000        | $B = 128$| 0.09900  | 0.0430| Yes       | 1.991 ± 0.031         | 1.009  |
| MNIST        | LeNet      | SGD       | 1000        | $B = 512$| 0.00787  | 0.0430| Yes       | 1.894 ± 0.028         | 1.119  |
| MNIST        | LeNet      | SGD       | 1000        | $B = 640$| 0.0125   | 0.0430| Yes       | 1.838 ± 0.027         | 1.194  |
| MNIST        | LeNet      | SGD       | 1000        | $B = 768$| 0.278    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | $B = 1024$| 0.129    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | $B = 8192$| 0.240    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | $B = 16384$| 0.249    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | $B = 32768$| 0.201    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | $B = 50000$| 0.139    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | $B = 60000$| 0.0936   | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | 40% Label Noise | 0.180    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | 80% Label Noise | 0.157    | 0.0430| No        |                       |        |
| MNIST        | LeNet      | SGD       | 1000        | Random Labels | 0.0482   | 0.0430| No        |                       |        |
| Fashion-MNIST| LeNet      | Random    | 1000        | -       | 0.0971   | 0.0430| No        | 1.939 ± 0.030         | 1.065  |
| Fashion-MNIST| LeNet      | SGD       | 1000        | -       | 0.0132   | 0.0430| Yes       | 1.550 ± 0.017         | 1.817  |
| MNIST        | LeNet      | SGD       | 1000        | Eigengap | 0.0153   | 0.0430| Yes       | 1.520 ± 0.017         | 1.922  |
| Fashion-MNIST| LeNet      | SGD       | 1000        | Eigengap | 0.0240   | 0.0430| Yes       | 1.520 ± 0.017         | 1.922  |

B.2. Image classification on MNIST and Fashion-MNIST

Data Preprocessing For MNIST and Fashion-MNIST: We perform the common per-pixel zero-mean unit-variance normalization.

Hyperparameter Settings: We select the optimal learning rate for each experiment from $\{0.0001, 0.001, 0.01, 0.1, 1, 10\}$ for SGD and use the default learning rate for adaptive gradient methods. In the experiments on MNIST and Fashion-MNIST: $\eta = 0.1$ for SGD, Vanilla SGD, Adai, PNM, and Lookahead; $\eta = 0.1$ for Vanilla SGD; $\eta = 0.001$ for Adam, AMSGrad, AdaBound, Yogi, RAdam, and DiffGrad.

We train neural networks for 50 epochs on MNIST and 200 epochs on Fashion-MNIST. For the learning rate schedule, the learning rate is divided by 10 at the epoch of 40% and 80%. The batch size is set to 128 for MNIST and Fashion-MNIST, unless we specify it otherwise.

The strength of weight decay is default to $\lambda = 0.0005$ as the baseline for all optimizers unless we specify it otherwise.

We set the momentum hyperparameter $\beta_1 = 0.9$ for SGD and adaptive gradient methods which involve in Momentum. As for other optimizer hyperparameters, we apply the default settings directly.

B.3. Image classification on CIFAR-10 and CIFAR-100

Data Preprocessing For CIFAR-10 and CIFAR-100: We perform the common per-pixel zero-mean unit-variance normalization, horizontal random flip, and $32 \times 32$ random crops after padding with 4 pixels on each side.
We also randomly shuffle the labels of MNIST to produce MNIST with random labels, which has little knowledge behind the pairs of instances and labels.

### Hyperparameter Settings

We select the optimal learning rate for each experiment from \{0.0001, 0.001, 0.01, 0.1, 1, 10\} for SGD and use the default learning rate for adaptive gradient methods. In the experiments on CIFAR-10 and CIFAR-100: \( \eta = 1 \) for Vanilla SGD, Adai, and PNM; \( \eta = 0.1 \) for SGD (with Momentum) and Lookahead; \( \eta = 0.001 \) for Adam, AMSGrad, AdaBound, Yogi, RAdam, and DiffGrad. For the learning rate schedule, the learning rate is divided by 10 at the epoch of \{80, 160\} for CIFAR-10 and \{100, 150\} for CIFAR-100, respectively. The batch size is set to 128 for both CIFAR-10 and CIFAR-100, unless we specify it otherwise.

The strength of weight decay is default to \( \lambda = 0.0005 \) as the baseline for all optimizers unless we specify it otherwise. Recent work Xie et al. (2020a) found that popular optimizers with \( \lambda = 0.0005 \) often yields test results than \( \lambda = 0.0001 \) on CIFAR-10 and CIFAR-100.

We set the momentum hyperparameter \( \beta_1 = 0.9 \) for SGD with Momentum. As for other optimizer hyperparameters, we apply the default hyperparameter settings directly.

### B.4. Learning with noisy labels

We trained LeNet via SGD (with Momentum) on corrupted MNIST with various (asymmetric) label noise. We followed the setting of Han et al. (2018) for generating noisy labels for MNIST. The symmetric label noise is generated by flipping every label to other labels with uniform flip rates \{40\%, 80\%\}. In this paper, when we talk about label noise, we mean symmetric label noise.

We also randomly shuffle the labels of MNIST to produce MNIST with random labels, which has little knowledge behind the pairs of instances and labels.

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**Table 4.** The Kolmogorov-Smirnov statistics of LeNet on CIFAR-10 and CIFAR-100. The estimated power exponent \( \hat{\beta} \) and slope magnitude \( \hat{s} \) are also displayed.

| Dataset     | Model   | Training | Sample size | Setting | \( d_{ks} \) | \( d_{c} \) | Power-Law | \( \hat{\beta} \pm \sigma \) | \( \hat{s} \) |
|-------------|---------|----------|-------------|---------|--------------|--------------|------------|---------------------|--------|
| CIFAR-10    | LeNet   | Random   | 1000        | -       | 0.0663       | 0.0430       | No         | 1.968 ± 0.031       | 1.033  |
| CIFAR-10    | LeNet   | SGD      | 1000        | -       | 0.0279       | 0.0430       | Yes        | 1.935 ± 0.030       | 1.069  |
| CIFAR-10    | LeNet   | Vanilla  | 1000        | -       | 0.0276       | 0.0430       | Yes        | 1.806 ± 0.025       | 1.241  |
| CIFAR-10    | LeNet   | Adam     | 1000        | -       | 0.0269       | 0.0430       | Yes        | 1.786 ± 0.025       | 1.271  |
| CIFAR-10    | LeNet   | AMSGrad  | 1000        | -       | 0.0232       | 0.0430       | Yes        | 1.901 ± 0.028       | 1.110  |
| CIFAR-10    | LeNet   | AdaBound | 1000        | -       | 0.0184       | 0.0430       | Yes        | 1.806 ± 0.025       | 1.241  |
| CIFAR-10    | LeNet   | Yogi     | 1000        | -       | 0.0310       | 0.0430       | Yes        | 1.918 ± 0.029       | 1.090  |
| CIFAR-10    | LeNet   | RAdam    | 1000        | -       | 0.0347       | 0.0430       | Yes        | 1.911 ± 0.029       | 1.098  |
| CIFAR-10    | LeNet   | PNM      | 1000        | -       | 0.0358       | 0.0430       | Yes        | 1.964 ± 0.030       | 1.037  |
| CIFAR-10    | LeNet   | Lookahead| 1000        | -       | 0.0303       | 0.0430       | Yes        | 1.803 ± 0.024       | 1.236  |
| CIFAR-100   | LeNet   | Random   | 1000        | -       | 0.0944       | 0.0430       | No         | 1.908 ± 0.029       | 1.101  |
| CIFAR-100   | LeNet   | SGD      | 1000        | -       | 0.0315       | 0.0430       | Yes        | 1.903 ± 0.029       | 1.108  |
| CIFAR-100   | LeNet   | Vanilla  | 1000        | -       | 0.0379       | 0.0430       | Yes        | 1.903 ± 0.029       | 1.108  |

**Table 5.** The Kolmogorov-Smirnov statistics of FCN. The estimated power exponent \( \hat{\beta} \) and slope magnitude \( \hat{s} \) are also displayed.

| Dataset | Model       | Training | Sample size | Setting | \( d_{ks} \) | \( d_{c} \) | Power-Law | \( \hat{\beta} \pm \sigma \) | \( \hat{s} \) |
|---------|-------------|----------|-------------|---------|--------------|--------------|------------|---------------------|--------|
| Avila   | 2Layer-FCN  | SGD      | 50          | -       | 0.0683       | 0.176        | Yes        | 1.604 ± 0.085       | 1.656  |
| MNIST   | 1Layer-FCN  | Random   | 1000        | -       | 0.185        | 0.0430       | No         | 2.209 ± 0.038       | 0.827  |
| MNIST   | 1Layer-FCN  | SGD      | 1000        | -       | 0.241        | 0.0430       | No         | 2.209 ± 0.038       | 0.827  |
| MNIST   | 2Layer-FCN  | Random   | 1000        | -       | 0.129        | 0.0430       | No         | 2.209 ± 0.038       | 0.827  |
| MNIST   | 2Layer-FCN  | SGD      | 1000        | -       | 0.0112       | 0.0430       | Yes        | 2.209 ± 0.038       | 0.827  |
| MNIST   | 4Layer-FCN  | Random   | 1000        | -       | 0.0628       | 0.0430       | No         | 2.209 ± 0.038       | 0.827  |
| MNIST   | 4Layer-FCN  | SGD      | 1000        | -       | 0.0141       | 0.0430       | Yes        | 2.209 ± 0.038       | 0.833  |
The Power-Law Spectrum

Table 6. The Kolmogorov-Smirnov statistics of ResNet18. The estimated power exponent $\hat{\beta}$ and slope magnitude $\hat{s}$ are also displayed.

| Dataset  | Model    | Training | Sample size | Setting | $d_{bs}$ | $d_c$ | Power-Law | $\hat{\beta} \pm \sigma$ | $\hat{s}$ |
|----------|----------|----------|-------------|---------|---------|------|-----------|--------------------------|--------|
| CIFAR-10 | ResNet18 | Random   | 50          | -       | 0.334   | 0.176 | No        |                         |        |
| CIFAR-10 | ResNet18 | SGD      | 50          | -       | 0.0803  | 0.176 | Yes       | 2.146 ± 0.162           | 0.873  |
| CIFAR-10 | ResNet18 | Vanilla SGD | 50     | -       | 0.0891  | 0.176 | Yes       | 2.193 ± 0.169           | 0.838  |
| CIFAR-10 | ResNet18 | Adam     | 50          | -       | 0.0478  | 0.176 | Yes       | 2.062 ± 0.149           | 0.950  |
| CIFAR-10 | ResNet18 | AMSGrad  | 50          | -       | 0.0542  | 0.176 | Yes       | 2.041 ± 0.147           | 0.961  |
| CIFAR-10 | ResNet18 | AdaBound | 50          | -       | 0.0588  | 0.176 | Yes       | 2.029 ± 0.146           | 0.971  |
| CIFAR-10 | ResNet18 | Yogi     | 50          | -       | 0.116   | 0.176 | Yes       | 1.915 ± 0.129           | 1.092  |
| CIFAR-10 | ResNet18 | RAdam    | 50          | -       | 0.168   | 0.176 | Yes       | 1.794 ± 0.1112          | 1.259  |
| CIFAR-10 | ResNet18 | Adai     | 50          | -       | 0.103   | 0.176 | Yes       | 2.183 ± 0.167           | 0.845  |
| CIFAR-10 | ResNet18 | PNM      | 50          | -       | 0.138   | 0.176 | Yes       | 2.132 ± 0.160           | 0.884  |
| CIFAR-10 | ResNet18 | Lookahead | 50      | -       | 0.110   | 0.176 | Yes       | 2.098 ± 0.155           | 0.911  |
| CIFAR-10 | ResNet18 | DiffGrad | 50          | -       | 0.068   | 0.176 | Yes       | 2.055 ± 0.149           | 0.948  |
| CIFAR-100| ResNet18 | Random   | 50          | -       | 0.373   | 0.176 | No        |                         |        |
| CIFAR-100| ResNet18 | SGD      | 50          | -       | 0.108   | 0.176 | Yes       | 2.299 ± 0.184           | 0.770  |

Table 7. The Kolmogorov-Smirnov Test Statistics of Protein.

| Protein | Sample size | $d_{bs}$ | $d_c$ | Power-Law | $\hat{\beta} \pm \sigma$ | $\hat{s}$ |
|---------|-------------|----------|------|-----------|--------------------------|--------|
| 4HHB    | 1000        | 0.0145   | 0.0430 | Yes       | 2.008 ± 0.032           | 0.992  |

C. The Spectral Analysis of Proteins

The elastic network models are widely applied to predict and characterize the slow global dynamics of a wide range of proteins and bio-machineries (Bahar et al., 2010; Tang & Kaneko, 2020). By describing the proteins as mass-and-spring networks, the elastic network models can capture the functional motions of proteins with minimal computational resources by focusing on the movement of proteins nearby the native structure. The movements of the proteins are described as the linear vibrations around the energy minimum of the energy landscape. It is worth noting that the model is not applicable for the dynamics far from the energy minimum, such as protein folding and unfolding problems.

C.1. Anisotropic Network Model (ANM)

In this work, we employ a typical form of the ENM, Anisotropic Network Model (ANM), to calculate the vibrational spectrum of proteins (Atilgan et al., 2001; Bahar et al., 2010). Previous research has shown that not only can ANM accurately reproduce the movements of residues as determined by experiments, but the model also fits well with the data on protein structure evolution (Tang & Kaneko, 2021).

To introduce the model settings of ANM, let us first consider the sub-system consisting of two nodes (amino acid residues) $i$ and $j$ connected with a harmonic spring. The coordinates of the two nodes are $\vec{r}_i = [x_i, y_i, z_i]$ and $\vec{r}_j = [x_j, y_j, z_j]$, respectively; and their native-state coordinates are $\vec{r}_i^0 = [x_i^0, y_i^0, z_i^0]$ and $\vec{r}_j^0 = [x_j^0, y_j^0, z_j^0]$. When the equilibrium distance between them is given by $s_{ij}^0 = |\vec{r}_i^0 - \vec{r}_j^0| = \sqrt{(x_i^0 - x_j^0)^2 + (y_i^0 - y_j^0)^2 + (z_i^0 - z_j^0)^2}$, and the instantaneous distance is given by $s_{ij} = |\vec{r}_i - \vec{r}_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$, then the potential of such a sub-system can be given as:

$$V_{ij} = \frac{K}{2} (s_{ij} - s_{ij}^0)^2,$$

(21)
where \( \kappa \) denotes the spring constant. Then, around the energy minimum, the second-order derivative of the \( V_{ij} \) with respect to \( \vec{r}_i \) can be given as:

\[
\frac{\partial^2 V_{ij}}{\partial x_i^2} = \frac{\partial^2 V_{ij}}{\partial x_j^2} = \frac{\kappa}{s_{ij}} (x_j - x_i)^2,
\]

\[
\frac{\partial^2 V_{ij}}{\partial x_i \partial y_j} = \frac{\kappa}{s_{ij}} (x_j - x_i)(y_j - y_i).
\]

Therefore, the corresponding Hessian matrix entries \( H_{ij} \) can be given as:

\[
H_{ij} = -\frac{\kappa}{s_{ij}} \begin{bmatrix} x_j - x_i \\ y_j - y_i \\ z_j - z_i \end{bmatrix} [x_j - x_i, y_j - y_i, z_j - z_i].
\]

In this way, the \( 3N_{AA} \times 3N_{AA} \) Hessian \( H \) can be recognized as the direct sum of the \( 3 \times 3 \) Hessian matrix \( H_{ij} \) and \( N_{AA} \times N_{AA} \) elasticity matrix \( \Gamma \). That is, the \( 3N_{AA} \times 3N_{AA} \) Hessian matrix \( H \) can be recognized as an \( N_{AA} \times N_{AA} \) matrix with entries of \( 3 \times 3 \) matrices

\[
H_{ij} = -\frac{\kappa}{s_{ij}} \Gamma_{ij} \begin{bmatrix} x_j - x_i \\ y_j - y_i \\ z_j - z_i \end{bmatrix} [x_j - x_i, y_j - y_i, z_j - z_i].
\]

Here, matrix \( \Gamma \) is defined according to the residue-residue contact topology of the native structure. In ANM, only spatial-neighboring residues are considered to be connected. For a pair of amino acid residues (\( i \) and \( j \)), if their mutual distance \( r_{ij} \leq r_C \), then \( \Gamma_{ij} = -1 \); if \( r_{ij} > r_C \), then \( \Gamma_{ij} = 0 \); and for the diagonal elements, \( \Gamma_{ii} = -\sum_{j \neq i} \Gamma_{ij} = -k_i \), where \( k_i \) denote the degree of node \( i \). Note that in a graph theory perspective, matrix \( \Gamma \) is also known as the graph Laplacian (or the Kirchhoff matrix) of the residue-residue contact network. In ANM with homogenous contact strength (\( \kappa = 1 \)), the only control parameter is the cutoff distance \( r_C \). In the calculation, we take \( r_C = 9.0 \) Å.

For a protein consisting of \( N_{AA} \) amino acid residues, the total degrees of freedom is \( 3N_{AA} \). Among them, there are 6 degrees of freedom related to the rigid body motion, say, three-dimensional translational motions and three-dimensional rotation. Therefore, to fully describe the structural fluctuations of a protein, one need in total \( n = 3N_{AA} - 6 \) parameters.

C.2. From ANM to SGD: Thermal noise vs. structured noise

Although the energy landscape around a protein’s native state is similar to the loss landscape of a deep neural network, the corresponding noises are entirely different. Protein dynamics are driven by thermal noises, and deep learning is driven by structured noises. Due to these two types of noise, the Hessian matrix and the covariance matrix have different relationships.

For a protein molecule driven by the thermal noises, according to the Boltzmann distribution, the probability of a structure \( \Delta \vec{r} \) is given as:

\[
p(\Delta \vec{r}) \sim e^{-\frac{1}{2} \sum_{i,j=1}^{N_{AA}} \Delta \vec{r}_i \cdot H_{ij} \cdot \Delta \vec{r}_j},
\]

in which \( \Delta \vec{r}_i = \vec{r}_i - \vec{r}_i^0 \) and \( \Delta \vec{r}_j = \vec{r}_j - \vec{r}_j^0 \) are three-dimensional vectors describing the displacements of residues \( i \) and \( j \). It is worth noting that \( p(\Delta \vec{r}) \) is a multivariate Gaussian distribution with covariance matrix \( C \sim H^{-1} \), where \( C_{ij} = \langle \Delta \vec{r}_i \cdot \Delta \vec{r}_j \rangle \).

However, as discussed in the main text, for SGD, the covariance matrix is proportional to the Hessian matrix: \( C_{\text{sgd}}(\theta) \sim H(\theta) \). Due to this difference, it is the spectrum of the inverse (or pseudoinverse) of Hessian \( H^{-1} \) that should be applied to compare with the Hessian matrices in deep learning.

C.3. Similarities in Hessian spectrums

By diagonalizing the Hessian matrix \( H \), we can obtain all the nonzero eigenvalues and the corresponding eigenvectors describing the motions of the protein, i.e., \( H = V \Lambda V^\top \), in which the eigenvalues \( \Lambda = \text{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n] \) (\( \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \)) and eigenvectors \( V = [v_1, v_2, \ldots, v_n]^\top \).

Then, for the inverse Hessian \( H^{-1} \), its nonzero eigenvalues \( \sigma_i = 1/\lambda_i \), and \( \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \). In Fig. 3b, as an example, the rank-size distribution of \( \sigma_i \) vs \( i \) is plotted. Here, we normalize all the eigenvalues as \( \tilde{\sigma}_i = \sigma_i / \sigma_1 \). The estimated power


**Table 8.** The approximation $s \approx 1$ positively correlates with the size of protein.

| Estimated Parameter | $300 \leq 3N_{AA} \leq 1000$ | $1000 \leq 3N_{AA} \leq 3000$ | $3000 \leq 3N_{AA} \leq 6000$ | $3000 \leq 3N_{AA} \leq 6000$ |
|--------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| $\hat{\beta}$     | $1.976 \pm 0.143$               | $1.973 \pm 0.103$               | $2.004 \pm 0.080$               | $1.975 \pm 0.128$               |
| $\hat{s}$          | $1.050 \pm 0.175$               | $1.041 \pm 0.119$               | $1.002 \pm 0.084$               | $1.045 \pm 0.155$               |
| $d_{ks}/d_{c}$     | $0.304$                         | $0.292$                         | $0.317$                         | $0.300$                         |

exponent (slope magnitude) $\hat{s} = 0.992$ (corresponding to $\hat{\beta} = 2.008 \pm 0.032$). This result clearly demonstrates the similarity between the vibrational spectrum of proteins and the Hessian spectrum in deep learning.

**C.4. Protein Dataset**

In this work, we evaluated the vibrational spectrums of 9166 kinds of protein molecules from the Protein Data Bank (PDB) (Berman et al., 2000). The studied proteins have high-resolution and clean structures, are large enough, and have enough diversity. More precisely, the structures of these proteins were all determined via high-resolution X-ray diffraction ($\leq 2.0 \text{Å}$) without DNA, RNA, or hybrid structures involved. Their chain lengths (number of amino acid residues) are $100 \leq N_{AA} \leq 2000$. Their spectrums have no zero eigenvalues except for the six modes correspond to the translational and rotational motions. Every two proteins share less than 30% sequence similarity. We choose the $\lambda_{cutoff}$ as the top $\frac{1}{10}$ largest eigenvalue in each vibrational spectrum for corresponding proteins.

We present the KS statistics of the protein spectrums in Figure 8. Note that, if $d_{ks}/d_{c} < 1$, we would reject the null hypothesis and accept the power-law hypothesis. All of the protein spectrums successfully passed the power-law KS tests with $mean(\hat{s}) = 1.045$ ($mean(\hat{\beta}) = 1.975 \pm 0.128$). We also notice that $\hat{s} \approx 1$ holds even better for larger proteins, which is supported by Table 8.

**D. Supplementary Empirical Results**

We compared the spectrum computed via Power Iteration Algorithm and Lanczos Algorithm in Figure 9. It shows the spectrum via Power Iteration Algorithm is highly consistent with the spectrum via Lanczos Algorithm. It also demonstrates that the power-law spectrum is caused by the properties of deep learning rather than the stochasticity of Lanczos Algorithm.

We presented the power-law eigengaps on Fashion-MNIST in Figure 10. It shows that the power-law eigengaps on Fashion-MNIST are highly consistent with the power-law eigengaps on MNIST.

We presented the power-law spectrum of the covariance matrix of stochastic gradient noise of FCN on MNIST in Figure 18. As the inverses of the power-law variables are power-law, the covariance spectrum shows heavy-tail properties. It demonstrates that the heavy-tail property belongs to deep neural networks rather than SGD itself.

We presented the power-law spectrum of two-layer FCN on Avila Dataset in Figure 11. It shows that the power-law
The Power-Law Spectrum

Figure 9. The spectrum via Power Iteration Algorithm is highly consistent with the spectrum via Lanczos Algorithm. It also shows that the power-law spectrum is caused by the properties of deep learning rather than the stochasticity of Lanczos Algorithm.

Figure 10. The power-law Hessian eigengaps in deep learning. Model: LeNet. Dataset: Fashion-MNIST. Subfigure (a) displayed the eigengaps by original rank indices sorted by eigenvalues. Subfigure (b) displayed the eigengaps by rank indices re-sorted by eigengaps.

Figure 11. The spectrum of FCN on Avila Dataset. It shows that the power-law spectrum of neural networks may also exist in non-image datasets.
The Power-Law Spectrum

Figure 12. The power-law spectrums of ResNet18 on CIFAR-10. It shows that the power-law spectrum of neural networks may also exist in modern neural network architectures (ResNet) as well as simple CNNs/FCNs.

Figure 13. The power-law spectrums hold across optimizers. Moreover, the slope magnitude $\hat{s}$ is an indicator of minima sharpness and a predictor of test performance. Model: LeNet. Dataset: CIFAR-10.

The power-law spectrum of neural networks may also generally exist in non-convolution neural networks trained on a non-image dataset. Particularly, we note that the Avila Dataset has only ten attributes, including intercolumnar distance, upper margin, lower margin, exploitation, row number, modular ratio, interlinear spacing, weight, peak number, and modular ratio/interlinear spacing. These attributes are essentially different from the pixels in image datasets.

We presented the power-law spectrums of ResNet18 on CIFAR-10 in Figure 12. It shows that the power-law spectrums hold for ResNet, which is a representative of the modern neural network architectures, as well as simple CNNs/FCNs. Due to the GPU memory limit, we may only display the top 50 eigenvalues for ResNet18. However, the KS test still supports to accept the power-law hypothesis.

The spectrums of LeNet on CIFAR-10 trained via various optimizers are showed in Figure 13. Figures 14 and 15 shows that the slope magnitude $\hat{s}$ closely correlates with the largest Hessian eigenvalue and the Hessian trace.

Figure 16 shows that the small width of neural networks may also break the power-law spectrum like small depth. This also supports that overparameterization or large model capacity is necessary for the power-law spectrum.

We report the spectrums of large-batch trained ResNet18 on CIFAR-10 in Figure 17. It indicates that the phase transition behaviors of the spectrums with respect to batch size generally exist. However, it seems that Phase II and Phase III merge into one phase for ResNet18 on CIFAR-10.

The heavy-tail property of SGD has been a hot and arguable topic recently (Simsekli et al., 2019; Panigrahi et al., 2019; Gurbuzbalaban et al., 2021; Hodgkinson & Mahoney, 2021; Xie et al., 2021b; Li et al., 2021). Note that the power-law
Figure 14. The slope magnitude $\hat{s}$ closely correlates to the largest Hessian eigenvalue and the Hessian trace. Model: LeNet. Dataset: MNIST.

Figure 15. The slope magnitude $\hat{s}$ closely correlates with the largest Hessian eigenvalue and the Hessian trace. Model: LeNet. Dataset: CIFAR-10.

Figure 16. The spectrums are not power-law for neural networks with small width ($\sim 10$), but gradually become more power-law (more straight in the log-log plot) as the width increases. This may also suggest that the power-law spectrum depends on model capacity. Model: Two-layer FCN. Dataset: MNIST.
Figure 17. Batch size matters to the spectrum. Model: ResNet-18. Dataset: CIFAR-10. The sharp phase transition occurs in $1152 < B < 1280$.

Figure 18. The power-law spectrum of gradient noise covariance exist in deep learning for various batch sizes. Model: Fully Connected Network (FCN). Dataset: MNIST.
distribution is one of the most common heavy-tail distributions in the real world. We argue that the arguable heavy-tail property of SGD may depend on the power-law Hessian spectrum rather than SGD itself, as gradient noise covariance critically depends on the Hessian. We present the power-law spectrums of gradient noise covariance in Figure 18.

We presented the spectrum of learning with clean labels and random labels in Figure 19. The number of top outliers obviously increases, because random labels make the dataset more complex. However, even if the pairs of instances and labels have little knowledge, we still observe the power-law spectrum after the dozens of top outliers. This may suggest that, even if the labels are random, neural networks can still learn useful knowledge from the instances only.